COLUMN2 - A Computer Program for Simulating Migration

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COLUMN2
- A computer program for simulating migration

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Abstract. COLUMN2 is a 1D FORTRAN77 computer program designed for studies of the effects of various physicochemical processes on migration. It solves the solute transport equation and can take into account dispersion, sorption, ion exchange, first and second order homogeneous chemical reactions. Spacial variations of input pulses and retention factors are possible. The method of solution is based on a finite difference discretion followed by the application of the method of characteristics and two separate grid systems. This report explains the mathematical and numerical methods used, describes the necessary input, contains a number of test examples, provides a listing of the program and explains how to acquire the program, adapt it to other computers and run it. This report serves as a manual for the program.

INIS-descriptors: COMPUTERIZED SIMULATION, COMPUTER CODES, MANUALS, RADIONUCLIDE MIGRATION, SOLUTES, ABSORPTION, HYDROLYSIS, COMPLEXES, RISK ASSESSMENT, CHEMICAL REACTION KINETICS

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PREFACE

This report presents the latest developments in a computer program constructed at Risø National Laboratory in 1978 (Bo 1978) to deal with studies of the effects of various physicochemical processes on migration. The purpose is to present the code for the program COLUMN2 and the physical and chemical concepts and assumptions used in COLUMN2. This report also serves as a manual to the program and the general subject of chemical and transport modelling has not been treated in all detail.

The basic framework of the first COLUMN program (Bo 1978) has been maintained. However, the new COLUMN2 program has been made user-friendly in contrast to the first version. COLUMN2 is written in standard Fortran 77 and has easy-to-handle input routines and has been expanded to include second order kinetics.

1. INTRODUCTION

1.1. General

The purpose of this work was first to construct a numerical framework and then a computer program to aid in the study of the effects of various physicochemical processes on migration.

Simulation of the behaviour of geochemical barriers in connection with risk assessment is not the primary use of this program, since such simulations are most often very site-specific and require complex geometrical considerations in addition to the chemical. In other cases they are so simplified that they lack both specific geometrical and chemical features. In the latter case the aquifer in question is treated as the column and the chemistry as a general physicochemical retention. Such simplified simulations are very useful and often give results with the accuracy needed without requiring an excessive amount of time and work.

When complex physicochemical processes are expected a close examination of the effects on migration is needed before the description of the process in question can be included in a more complex geochemical barrier simulation.

For purposes like this, a one-dimensional description will be adequate and will at the same time be able to simulate laboratory column experiments that are part of fundamental experimental migration studies (Carlsen et al. 1981).

For radioactive substances the decay and the decay of radionuclide chains are important processes whose influence on the migration has been described earlier (Burkholder et al. 1974). These processes can also be studied with COLUMN2. However, it should be emphasized here that COLUMN2 by no means is specially coupled to treatment of radioactive substances, but includes general coupling with more complex physicochemical processes.

The PERCOL model (Routson and Serne 1972) does treat complex chemical processes, but only in an emperical manner as far as the microcomponents are concerned. This partly excludes the identification of the physicochemical processes involved in the retention of these substances. Furthermore, the model is site-specific in the sense that it includes only a limited number of variable chemical phenomena.

The original COLUMN program has been included and reviewed in a recent comprehensive directory of geochemical computer programs (Broyd et al. 1983).

1.2. Reactions that may influence the migration behaviour of solutes.

A wide range of geochemical processes involving possible pollutants, often present as microcomponents, in the terrestrial environment can be expected a priori to influence the migration behaviour of the latter. In principle, all processes can be regarded as more or less sophisticated combinatons of uni- and bimolecular reactions. However, in practice the majority of bimolecular reactions will involve the macrocomponents in the ground water, the concentrations of these being up to several orders of magnitude higher than those of the microcomponents under investigation. Hence, these reactions can be treated as pseudo first-order reactions with respect to the micro components. In Table I the different elementary reactions that should be taken into account are summarized.

Table I. Characterization of elementary reactions, which may influence the migration. (FO: first-order, PFO: pseudo first-order, SO: second order)

Reaction	Type	Forward	Backward
Radioactive Decay Chains	$A \rightarrow B \rightarrow \cdots\cdots \rightarrow C$	FO	-
Sorption/Desorption	$A \rightleftarrows B$	FO	FO
Precipitation/Dissolution	$A \rightleftarrows B$	FO	FO
Redox Reactions[a]	$A \rightleftarrows B$	PFO	PFO
Degradations	$A \rightarrow \Sigma B_i$	FO	-
-	$A+X \rightarrow \Sigma B_i$	SO/PFO	-
Substitutions[b]	$A+X \rightarrow B$	SO/PFO	-
Hydrolysis	$A+OH \rightarrow B$	PFO	-
Complex Formation[c]	$A+L \rightleftarrows AL$	SO/PFO	FO
Colloid Formation[d]	$nA \rightarrow A_n$	SO	-

[a] The redox potential will generally be controlled by the macro composition of the ground water (e.g. by the Fe(II)/Fe(III) couple)

[b] The substitution reactions may be of importance in cases of organic pollutants

[c] In the case of complex formation, which can be expected to influence the migration behaviour of metal cations significantly, it is to be expected that in most cases it can be treated as a PFO reaction, owing to a large excess of the ligand, or a constant concentration of the latter (e.g. naturally occurring ligands in ground water).

[d] Colloid formation can in principle be regarded as a consecutive series of SO reactions.

Numerous combinations of the above mentioned elementary reactions can be imagined. Especially parallel reactions, e.g. as a result of concurring chemical and microbiological transformations, and consecutive reactions, e.g. hydrolysis subsequently followed by a

precipitation/dissolution reaction of the hydrolyzed species, shall be mentioned.

2. MATHEMATICAL DESCRIPTIONS

2.1. Convection and dispersion

Common to all the solutes present in the liquid phase is the transport due to convection and dispersion which we describe by:

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} - V \frac{\partial c_i}{\partial x} \qquad (1)$$

where c_i is the concentration of component i.
D_i is the dispersion coefficient of component i.
V is the interstitial velocity of the liquid phase ($V = q/\epsilon$)
q is the volume flow per unit cross-sectional area.
ϵ is the porosity (volume fraction of liquid) of the porous medium.
t is the time.
x is the length coordinate.

Equation (1) assumes that neither the dispersion nor the interstitial velocity changes in the x-direction. Most often the interstitial velocity will be so high that all components have the same dispersion coefficient, but at very low velocities differences between the individual components do occur as a result of their individual diffusion coefficients in the liquid phase.

It sometimes happens that it is necessary to account for a component that does not move with the fluid flow, e.g. precipitates and absorption in the solid phase under non-equilibrium conditions. This can be done by setting the dispersion coefficient and the interstitial velocity equal to zero for such components.

2.2. Equilibrium adsorption/absorption phenomena

2.2.1. General description

When, in addition to dispersion and convection, components are transferred between the liquid (flowing) and the solid (stationary) phases, the transport equation (1) is modified by adding a term which describes the effect of these processes on the concentration in the liquid phase:

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} - V \frac{\partial c_i}{\partial x} - \frac{\varepsilon_s}{\varepsilon} \frac{\partial \bar{c}_i}{\partial t} \qquad (2)$$

where $\bar{c}_i$ is the concentration of i in the solid phase, and ε_s is the volume fraction of the solid phase. If the process is an adsorption on a surface, ε_s and $\bar{c}_i$ has the meaning of specific surface area and surface concentration, respectively.

The form of equation (2) is especially useful for fast reversible reactions in which equilibrium between the liquid and solid phases can be assumed at all times, because in this case

$$\frac{\partial \bar{c}_i}{\partial t}$$

does not depend explicitely on time, but can be expressed in terms of c_j and

$$\frac{\partial c_i}{\partial t}$$

which relates only to the liquid phase, i.e. when

$$\bar{c}_i = f_i(c_j, \ldots\ldots) \qquad (3)$$

then

$$\frac{\partial \bar{c}_i}{\partial t} = \sum_i \frac{\partial f_i(c_j,.....)}{\partial c_1} \frac{\partial c_1}{\partial t} \qquad (4)$$

Expressions such as (3) and (4) gives rise to the distinction between micro-chemistry (micro-components) and macro-chemistry (macro-components) because very often a few components completely determines the value of the functions $f_i(c_j,....)$ because of their relatively large concentrations. This is true also for components i present in small (micro) concentrations. Use of expressions like (3) and (4) requires, however, that the components i are present in amounts that makes their properties thermodynamically well defined, i.e. not subject to statistical fluctuations that are too large. This leaves us with a third category - submicro-chemistry - that cannot be treated by thermodynamics. Instances of the importance of this type of component may be found in the migration of some radionuclides. These problems will, however, not be treated here.

2.2.2. Ion Exchange

Ion exchange is one of the more important mechanisms by which positively charged ions are retained in soil. The exchange process is relatively rapid and reversible. Therefore the assumption of maintaining equilibrium at all times during the migration is most often fulfilled.

The equilibrium is determined by the equality of the electro-chemical potentials in the ion exchange phase and in the liquid phase for each of the components present. Expressed in terms of concentrations this equilibrium can be written:

$$\bar{c}_i = c_i \frac{\gamma_i}{\bar{\gamma}_i} K_i Z^{z_i/\omega} \qquad (5)$$

where

$$Z = \exp(\omega F(\psi - \bar{\psi})/RT) \qquad (6)$$

$$K_i = \exp((\mu_i^{\circ} - \bar{\mu}_i^{\circ})/RT) \qquad (7)$$

and
- γ_i is the activity coefficient of component i
- z_i is the valence factor of the component i
- ω is the change factor for the fixed ions in the exchange phase (-1 for a cation exchanger)
- μ_i° is the standard chemical potential of component i
- ψ is the electrical potential of the phases
- F is Faradays number
- R is the gas constant
- T is the absolute temperature
- a bar ($\bar{}$) over a symbol refers to a property in the ion exchange phase.
- K: distribution coefficient
- Z: potential function

Z is determined by the condition of electroneutrality in the ion exchange phase:

$$\sum_j z_j \bar{c}_j + \omega X = o \qquad (8)$$

where X is the concentration of the fixed ionic groups in the exchanger phase. Inserting (5) in (8) gives a polynomial expression in Z which can be solved when the constants and the concentrations in the liquid phase are known.

With the above expressions for the equilibrium we find:

$$\frac{\partial \bar{c}_i}{\partial t} = K_i \frac{\gamma_i}{\bar{\gamma}_i} Z^{z_i/\omega} \frac{\partial c_i}{\partial t} + \frac{z_i}{\omega} c_i K_i \frac{\gamma_i}{\bar{\gamma}_i} Z^{z_i/\omega} \frac{\partial \ln Z}{\partial t}$$

which with

$$K_{Di} = K_i \frac{\gamma_i}{\bar{\gamma}_i} Z^{z_i/\omega} \qquad (9)$$

gives

$$\frac{\partial \bar{c}_i}{\partial t} = K_{Di} \frac{\partial c_i}{\partial t} + \frac{z_i}{\omega} c_i K_{Di} \frac{\partial \ln Z}{\partial t} \qquad (10)$$

When inserted into the migration Eq. (2) with

$$A_i = 1 + K_{Di} \frac{\varepsilon_s}{\varepsilon} \tag{11}$$

where A_i is inverse retention factors, we get

$$\frac{\partial c_i}{\partial t} = \frac{D_i}{A_i} \frac{\partial^2 c_i}{\partial x^2} - \frac{v}{A_i} \frac{\partial c_i}{\partial x} - c_i \frac{A_i - 1}{A_i} \frac{\partial \ln Z}{\partial t} \tag{12}$$

in which

$$\frac{\partial \ln Z}{\partial t}$$

can be expressed in terms of

$$\frac{\partial c_j}{\partial t}$$

through

$$\frac{\partial \ln Z}{\partial t} = \sum_i \frac{1}{Z} \frac{\partial Z}{\partial c_j} \frac{\partial c_j}{\partial t}$$

or using the electroneutrality condition in the form

$$\sum_j z_j \frac{\partial \bar{c}_j}{\partial t} = 0 \ .$$

The microchemistry, i.e. the components that need not be considered when calculating Z, can often be described by the simplified equation:

$$\frac{\partial c_i}{\partial t} = \frac{D_i}{A_i} \frac{\partial^2 c_i}{\partial x^2} - \frac{v}{A_i} \frac{\partial c_i}{\partial x} \tag{13}$$

However, this requires either that the macrochemistry (and therefore Z) be independent of time or A_i be very close to 1.

Finally it should be mentioned that neither Z nor the individual K_i's are thermodynamically well defined and, in the actual calculation, should be replaced by products and ratios of these parameter that are thermodynamically well defined.

2.2.3. Other types of sorption

When the sorption isotherm is known:

$$\bar{c}_i = f_i(c_j, \ldots\ldots) \tag{3}$$

as a function of all components present, the time derivative can be found

$$\frac{\partial \bar{c}_i}{\partial t} = \frac{\partial f_i(c_j, \ldots.)}{\partial c_l} \frac{\partial c_l}{\partial t} \tag{4}$$

$$\text{Defining } K_{Di} = \frac{f_i(c_j, \ldots..)}{c_i} \text{ and } A_i = 1 + \frac{\varepsilon_s}{\varepsilon} K_{Di} \tag{14}$$

We get the transport equation:

$$\frac{\partial c_i}{\partial t} = \frac{D_i}{A_i} \frac{\partial^2 c_i}{\partial x^2} - \frac{v}{A_i} \frac{\partial c_i}{\partial x} + \frac{A_i - 1}{A_i} \frac{\partial c_i}{\partial t}$$

$$- \frac{\varepsilon s}{\varepsilon} \sum_l \frac{\partial f_i(c_j, \ldots.)/\partial c_l}{A_i} \frac{\partial c_l}{\partial t}. \tag{15}$$

This again takes the form (13) if for all $l \neq i$ either

$$\frac{\partial f_i(c_j, \ldots.)}{\partial c_l} = 0 \text{ , or } \frac{\partial c_l}{\partial t} = 0 \text{ , and for } l = i$$

$$\frac{\partial f_i(c_j, \ldots.)}{\partial c_l} = \frac{f_i(c_j, \ldots..)}{c_i} \text{ .}$$

The first and last condition is likely to hold true for many microcomponents whereas the second will sometimes be a good approximation for macrocomponents.

2.3. First order reactions in solution and radioactive decay

Homogeneous chemical reactions and that part of heterogeneous reactions that concerns dissolved species and radioactive decay are introduced into the transport equation by adding terms of the form

$$\sum_l \prod_j S_{ij}^l \, c_j^{a(l,j)}$$

where l represents the chemical reaction in question and j is a component in this reaction which enters the reaction rate for component i with the coefficient S_{ij}^l and the exponent a(l,j).

For first order reactions and radioactive decay the above expression simplifies to

$$\sum_l S_{il} \, c_l$$

since, in this case, the reaction can be identified with the component involved in the reaction. This expression gives a transport equation of the form:

$$\frac{\partial c_i}{\partial t} = \frac{D_i}{A_i} \frac{\partial^2 c_i}{\partial x^2} - \frac{v}{A_i} \frac{\partial c_i}{\partial x} + \sum_l \frac{S_{il}}{A_i} \qquad (16)$$

in which also retention due to sorption, in its simplest form, has been taken into account.

Since

$$S_{il} = \left(\frac{\partial c_i}{\partial t}\right)^l \frac{1}{c_l} \qquad (17)$$

where the superscript l means that part of the derivative that is due to the reaction l, S_{il} is, for a simple chemical reaction, a normal rate constant.

For radioactive decay, which is going on both in the liquid and solid phases

$$S_{il} = \lambda_l + \lambda_l \frac{\varepsilon_s}{\varepsilon} K_{Dl} = \lambda_l A_l \qquad (18)$$

where λ_l is the decay constant - taken positive for parent radionuclides ($l \neq i$) and negative for the component i itself. The two terms in the middle part of (18) arises because of decay in the liquid phase and of reestablishing of equilibrium between and solid phase following decay in the solid phase.

An other important application of these equations is to pseudo-first order reactions in which e.g. a complexing agent (L^{z_l}) reacts with positively charged ions (M^{z_m}) to form another charged species

$$M^{z_m} + L^{z_l} \rightleftharpoons ML^{z_m+z_l} \qquad (19)$$

with a retention (A_i) different from the simple ion. When the concentration of the complexing agent is high compared with the concentration of the ion M^{z_m}, the reactions (19) can be treated as first order reactions. Hydrolysis and precipitation of micro-components in a buffered system or one in which the concentration of the precipitating component is high compared with the concentration of the microcomponent can also, at least to a certain extent, be treated as first order reactions.

2.4. Second order reactions in solution

The second order reactions are not introduced directly into the transport equation but treated seperately. Terms of the form

$$SR_r \times R1_r \times R2_r \times dt$$

are subtracted and added, respectively, to the concentrations of the relevant components for each reaction, r, where

SR_r is the second order rate constant
$R1_r$ is the concentration of the first reactant
$R2_r$ is the concentration of the second reactant.

3. NUMERICAL METHODS

3.1. Introduction

When making a program for the calculation of migration phenomena, a choice must be made: should we plan a large program, comprising all possible phenomena, in which the problem to be studied in each specific case is selected in the input, leaving the program proper unmodified at all times ? Or skould we plan a program comprising only the basic scheme common to all the individual problems to be solved, leaving the user of the program modify it according to his needs.

For the following two reasons we have chosen the second of the above-mentioned alternatives:

1) We cannot possibly foresee all the problems, hopefully to be solved with the program, and their numerical peculiarities
2) Solving specific detail problems with an all comprising program is often a waste of computer time, and will often leave the user in doubt as to whether the program function, all right for the specific problem thus necessitating a number of test calculations with the large program.

3.2. Convection and Dispersion

Setting up algorithms to solve Eq. (1) for one dimensional transport by convection and dispersion, we have to choose: (a) between finite difference and finite elements methods, and (b) between explicite and implicite algorithms. The criteria for the

choice should be both ease of handling modifications of the program, and minimizing the computer time needed for the problems. This, in our opinion, leads to choose finite difference explicite algorithms. They are the easiest to modify but not necessarily the fastest for calculation. However, the use of a modified method of characteristics to solve the hyperbolic part of the problem ($V\partial c_i/\partial x$) to some extent compensates for this.

Using methods of characteristics, Eqs. (1) or (13) is rearranged thus:

$$\frac{dc_i}{dt} = \frac{\partial c_i}{\partial t} + \frac{V}{A_i}\frac{\partial c_i}{\partial x} = \frac{D_i}{A_i}\frac{\partial^2 c_i}{\partial x^2} \qquad (20)$$

where the substantial derivative on the left is the concentration change in a local liquid volume that follows the movement (V/A_i) of the component i in the liquid phase. In this way the stability problem with the otherwise hyperbolic equation is circumvented - but it necessitates the introduction of a set of grid points (space points at which concentrations etc. are calculated) that are moving with the velocity V/A_i relative to the stationary phase - i.e. the column. In many applications of the method of characteristics the actual numerical integration is, however, performed on an equidistant stationary set of grid points. This gives the following integration cycle:

1) Calculate the concentrations at the fixed grid points from the values at the moving points. This is done by averaging over flowing grid points that are within half a fixed grid point interval form a given fixed grid point.
2) Perform the numerical integration on the equidistant fixed grid points.
3) Calculate the new concentrations on the moving grid points by adding the increment found in 2) for each of the fixed grid points, to all the moving grid points within half a fixed grid point interval from the given fixed grid point.
4) Move the flowing grid points by adding to their corresponding x-values - V/A_i times the time increment.

On the average this calculating procedure gives very accurate results but has a tendency to give local (in space) errors when sharp concentration profiles on the moving grid point pass a fixed grid point.

The logical way to remove these difficulties is to dispense with the fixed grid points and perform the integration on the moving grid points. This makes the integration cycle consist of only two operations:

1) Perform the integration on the moving grid points.
2) Move the grid points by adding V/A_i times the time increment to their x-values, thus keeping track on the whereabouts of the different components.

This sounds as a greater simplification than it actually is because of two types of phenomena:

The first is that A_i may vary explicitly or implicitly with x-coordinate in the column making flowing grid points crowd at some places and spread at others. This necessitates an integration procedure that is able to work with grid points that are not equidistant.

The second is that when the different components are coupled e.g. through chemical reactions in the liquid phase, and they do not move at the same speed relative to the stationary phase, then one components concentration has to be calculated at other components grid points. This is done by interpolation.

The first order finite difference representation of first and second order spatial differential coefficients for nonequidistant grid points, as used here, are:

$$\left(\frac{\partial c}{\partial x}\right)_{x(L)} = c'_L = \frac{1}{2}\left(\frac{c_{L+1} - c_L}{h_{L^+}} + \frac{c_L - c_{L-1}}{h_{L^-}}\right) \qquad (21)$$

$$\left(\frac{\partial^2 c}{\partial x^2}\right)_{x(L)} = c_L'' = \frac{2}{h_{L+} + h_{L-}} \left(\frac{c_{L+1} - c_L}{h_{L+}} - \frac{c_L - c_{L-1}}{h_{L-}}\right) \quad (22)$$

Both reduce to first order central differences approximations for $h_{L+} = h_{L-}$. The terminology can be inferred from Fig. 3.1. For simplicity of exposition the component identification subscript has been omitted.

Using a forward difference for the time derivative:

$$\left(\frac{dc}{dt}\right)_{x(L)} = \frac{c_{L,n+1} - c_{L,n}}{k} \quad (23)$$

where n enumerates the time and k is the time interval, and introducing the abreviation:

$$H = \frac{2\ h_{L-}}{h_{L+} + h_{L-}}$$

we get for the differential equation:

$$\frac{dc}{dt} = \frac{D}{A} \frac{\partial^2 c}{\partial x^2}$$

the explicite finite difference expression:

$$c_{L,n+1} = c_{L,n} + \frac{D-k}{A \times h_{L+} \times h_{L-}} (H(c_{I+1,n} - c_{L,n}) -$$

$$(2-H)\ (c_{L,n} - c_{L-1,n})) \quad (24)$$

from which the concentration profile at time (n+1)k can be calculated from the profile at time n+k.

At the boundary x=0, the input concentration to the column must be specified as a function of time i.e. $c_o = g(t)$. This is the mathematical boundary condition at this point. Since integration will be made between grid points normally, and since we cannot be sure whether we have a grid point at x=0 or not, the inte-

gration for the first point in the column, i.e. with X(I,J+1):

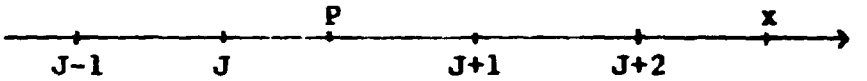
is made using (24) but substituting x=0 and c_o for the point at L-1.

At the end of the column of length P, i.e. at x=P the mathematical boundary condition is:

$$(\frac{\partial c}{\partial x})_P = 0 \ .$$

Since we do not always have a grid point at x=P we have to make an interpolation:

$$c'_P = c'_J + (P - x_J)(c'_{J+1} - c'_J)/(x_{J+1} - x_J) = C.$$



which results, using (21), in the following expression for $c_{J+2,n+1}$:

$$c_{J+2,n+1} = c_{J+1,n+1} - \frac{x_{J+2} - x_{J+1}}{P - x_J}(c_{J+1,n+1} - c_{J,n+1})$$

$$+ \frac{P - x_{j+1}}{P - x_J} \frac{x_{J+2} - x_{J+1}}{x_J - x_{J-1}} (c_{J,n+1} - c_{J-1,n+1}) \qquad (25)$$

This means that the normal integration using (24) must be carried out up to and including the grid point J+1.

3.3. Equilibrium sorption phenomena

For ion exchange and other equilibrium sorption phenomena, A_i is calculated in a subroutine prepared especially for the specific problem at hand.

As seen from Eqs. (12) and (15) it is sometimes necessary to solve a set of partial differental equations that are coupled through their partial time derivatives (not through the substantial time derivatives). The correct way to solve this problem would be to solve the resulting m equations in m unknown partial time derivatives ($\partial c_i/\partial t$). Such a procedure does not fit into the general scheme used here, where only the substantial derivative is calculated. It is furthermore likely to give stability problems because of the mixed parabolic ($\partial^2 c_i/\partial x^2$) and hyperbolic ($\partial c_i/\partial x$) nature of the set of equations that result from considering the partial time derivatives as the unknowns.

An approximation that is numerically easier to handle is to substitute the value of the partial time derivatives that can be calculated from the known concentration profiles at time (n-1)×k and n×k - for the ones that appear on the right side of (12) and (15) and should correspond to the time interval n×k to (n+1)×k. This adds to the right side of (24), considered to describe the concentration of component i, a term of the form:

$$\sum_j Q_{ij} \times k \times (c_{j,x_i(L),n} - c_{j,x_x(L),n-1}) \qquad (26)$$

where the subscript "$x_i(L)$" means that the concentration of component j should be evaluated at this x-value which is a grid point for component i but most often not for component j when j ≠ i. In the same way Q_{ij}, whose meaning depends on the specific problem to be solved, should be evaluated at the same place.

3.4. Chemical reactions in solution and radioactive decay

First order chemical reactions in solution and radioactive decay adds to the right side of (24) a term of the form:

$$\sum_i \frac{S_{il} - k}{A_i} c_{l,x_i(L),n}$$

where the meaning of S_{il} for the different processes has already been discussed.

3.5. Solid phase reactions

When non-equilibrium sorption processes, precipitation or other processes, in which the amount of a component in the solid phase is not determined solely by the concentrations that, at the time of interest, exists in the liquid phase, then it is necessary to keep track on the amount of this component. This is because, it is impossible to dissolve as precipitate that is no longer there! If the transfer of the component in question, back to solution, is not in some way proportional to a positive power of the concentration in the solid phase, then logical statements has to decide whether, at a given time and place, it is possible to transfer more of the component from the solid to the liquid phase. The meaning of "concentrations" and possibly ε_s has to be redefined according to the needs in each specific case. The fact that such components do not move with the liquid phase is taken care of by setting the interstitial liquid velocity (for these components only) and their dispersion coefficients equal to zero.

4. DESCRIPTIONS OF INPUT

COLUMN2 is designed to perform only one simulation in a single computer run. The program reads the input from a diskfile, file 1 with the name IFILE.

A special program, COLUMNINPUT, has been constructed to set up input files in a very easy way. COLUMNINPUT uses a finite automatic table generator system (FATGS) for manipulation of input. An input file can be constructed interactively starting from scratch. Or you can enter one input file already constructed, modify the input, and save it as another input file on disk. This is very useful when doing long series of parameter studies. COLUMNINPUT has been listed in appendix III.

All input are read in free field format. Required input begins with a title card followed by an output option card. The program can be run both interactively, which means that output plots are obtained on a graphics terminal, or in batch mode, which means that you will submit the run as a job and get the output plot on some external plotter, e.g. lineprinter or calcomp plotter or stored in a plotfile for later inspection. The present version of COLUMN2 uses a very strong computer grafics system developed at Risø Computer Installation (Rahbek and Hansen, 1983) for handling plotting. However, a version containing only a simple lineprinter option is available on request to the authors. In the input cards remember that input reals have to contain a decimal point. Examples of input will be given in Chapter 6.

1. TITLE, Title
   maximum 36 characters

2a PLNAC, Name for the concentration plot, maximum 6 characters

2b PLNAE, Name for the effluent plot, maximum 6 characters.

3. Output options, (IOUT(I), I = 1,3)

   IOUT(1) = 0 , print of input
   IOUT(1) = 1 , no print of input

   IOUT(2) = 0 , allows the amount of computing time stated in job card
   IOUT(2) = 1 , allows a maximum of 300 seconds computing time
   IOUT(2) = 2 , allows a maximum of 60 seconds computing time

   IOUT(3) = 0 , negative concentrations are set equal to zero
   IOUT(3) = 1 , negative concentrations are carried on in calculations

   IOUT(4) = 0 , integration of each component is carried out
   IOUT(4) = 1 , no integration of peaks

IOUT(5) = 0 , hardcopy plot in batch job
IOUT(5) = 1 , no hardcopy plot in batch job

4. N, number of components
5. M, number of points uneven integer less than 801
6. P, length of column
7. II, number of timesteps between outputting a concentration profile
8. III, number of timesteps between outputting an effluent profile
9. V, velocity
10. TMAX, maximum time
11. DCINT, integration constant - should be fixed at 100000
12. DELTAT, time between integration steps
13. Input options (IOPT(I), I = 1,7)

IOUT(I) = 0 , *different parameters for different components*
= 1 , all parameters, e.g. D, equal for all component
I = 1 : D
I = 2 : retention factors
I = 3 : minium value on y-axis for concentrations
I = 4 : maximax value on y-axis for concentrations
I = 5 : minimum value on y-axis for effluents
I = 6 : maximum value on y-axis for effluents
I = 7 : first order rate constant.

14. D, dispersion coefficients
15. AS, AE, retention factor at the start and end of the column
16. YCMIN, minimum value on y-axis for concentrations
17. YCMAX, maximum value on y-axis for concentrations
18. YEMIN, minimum value on y-axis for effluents
19. YEMAX, maximum value on y-axis for effluents
20. INSR, number of second order reactions
21. R1, R2, P1, P2, SR, number of reactant 1
number of reactant 2
number of product 1
number of product 2
second order rate constants
22. S(i,j), first order rate constants for components i to j. S(j,i) is -S(i,j)

23. Concentration input options, (ICIN(I), I = 1,N)
    ICIN(I) = 0 continuous flow through column
    ICIN(I) = 1 time-limited input pulse
    ICIN(I) = 2 point-limited input pulse

24a. IFORM(I), COTIME(I), CO(I)
     IFORM(I) = 0 constant input
     IFORM(I) = 1 variable input that must be specified
     CONTIME(I),   time the pulse lasts
     CO(I)   , value of the input concentration

24b. IFORM(I), IENPOI(I), ISTPOI(I)
     IENPOI(I), endpoint of pulse (highest number)
     ISTPOI(I), startpoint of pulse (lowest number)

25. C(III,I,ISTPOI(I)), input concentration

5. PROGRAM LIMITATIONS

As already indicated COLUMN2 is an extremely general program. The limitations lie in the dimensioning of arrays. For computational reasons the number of components has been limited to 5 and a maximum number of 10 second order reactions. However, a redimensioning of all relevant arrays will allow for any number of components and reactions desired. Arrays should never be dimensioned larger than needed in order to save computation time. 5 components and 10 second order reactions may seem as small numbers. However, larger simulations are often divided into smaller subproblems for clarification purposes. The maximum number of grid points has been set to 801. This number can also be enlarged by a redimensioning of relevant arrays which causes longer computation times.

6. TEST EXAMPLES

6.1. Introduction

The following test examples have been designed not only to illustrate how to set up input files but also to show the output and check the program in different ways. For each test example the input file is listed and the resulting plots from COLUMN2 are listed. This may be useful for comparison purposes in making COLUMN2 operate on other computer installations. The results are discussed briefly.

6.2. Test example 1

This test example which is probably the simplest one can think of is made as a test of the numerical accuracy.

Input data:
```
 100 TEST CASE NO. 1
 200 PLOT1C
 300 PLOT1E
 400 1,2,1,1
 500 1
 600 401
 700 100
 800 10
 900 1
1000 1.0
1100 100.0
1200 100000
1300 2
1400 1,1,1,1,1,1,1
1500 0.03
1600 1.,1
1700 0
1800 1
1900 0
```

```
2000 1
2100 0
2200 0
2300 2
2400 0,240,236
2500 1.535
```

There is one component present. 401 grid points are used giving initially 200 grid points inside the column whose length is 100 m. The interstitial velocity is 1 m/year and the dispersion-coefficient is 0.03 m^2/year corresponding to the diffusion coefficient in water, that is, the lowest possible.
There are no reactions going on. The timestep is 2 years and concentration profiles are collected for every 10 time steps and effluent concentration for each time step. The initial concentration profile is square from grid points 246 to 240, with a concentration of 1.535 moles/m^3. The retention factor is equal to 1 all over the column which corresponds to no absorption on the solid phase. In Fig. 6.1 the output of this test example is shown.

For this test example there exists an analytical solution:

$$c = 1/2\ c_o\ (\mathrm{erf}((h-x)/2\sqrt{Dt}) + \mathrm{erf}((h+x)/2\sqrt{Dt}) \quad ,$$

where erf is the error function, h is the half width of the initial concentration profile. The analytical solution is plotted on top of the output in Fig. 6.1. No difference between the numerical and the analytical solution is seen.

6.3. Test example 2

In this test example a retention factor that varies linearly with distance in the column is introduced. It varies from 1 at the entrance to 3 at the exit of the column:

$$A(I,L) = 1. + 2 \cdot X(I,L)/P \ .$$

Input data:

```
 100 THIS IS TEST CASE NO. 2
 200 PLOT2C
 300 PLOT2E
 400 1,2,1,1
 500 2
 600 401
 700 100
 800 10
 900 1
1000 1.0
1100 250.0
1200 100000
1300 2
1400 1,0,1,1,1,1,1
1500 0.03
1600 1.,3.,1.,3
1700 0
1800 1
1900 0
2000 1
2100 0
2200 0
2300 2,0
2400 0,200,196
2500 1.535
2600 1.
```

The input data are the same as in the previous example, except for the number of components, namely, two chemically independent ones. Component 1 has a square input concentration profile from grid point 196 to 200 just in front of the column while 2 has a continous input with a concentration equal to 1 mole/m^3. From part of the terminal written output:

```
REDISTRIBUTION AT T=      0.8000E+02
REDISTRIBUTION AT T=      0.8000E+02
REARRANGEMENT OF X-AXES AT T=      0.9800E+02
REARRANGEMENT OF X-AXES AT T=      0.9800E+02
REDISTRIBUTION AT T=      0.1600E+03
REDISTRIBUTION AT T=      0.1600E+03
REARRANGEMENT OF X-AXES AT T=      0.1840E+03
REARRANGEMENT OF X-AXES AT T=      0.1840E+03
REDISTRIBUTION AT T=      0.2400E+03
REDISTRIBUTION AT T=      0.2400E+03
```

It is seen the two different operations on the grid points have been performed: (a) It has been necessary to redistribute the grid points every 80 years because the distance between some of the grid points gets too small. The faster-moving points at the beginning of the column approach the slower-moving ones at the end of the column. (b) It has also been necessary to rearrange the x-axis every 90 years because the first grid point gets too close to x=0 and many of grid points have left the column at the other end.

Figure 6.2 shows the plotted output. It is seen that the peaks lie closer and closer to each other due to the linearly increasing value of A. From the eluate plot it is seen that both the peak of component 1 and the half-maximum value of 2 both occur at T=200 years corresponding to a mean value of A equal to 2.

6.4. Test example 3A

In this and the five following test examples the algorithm for first and pseudo first order reactions is tested. Component 1 has retention A(1) = 2 due to e.g. ion exchange. It reacts with a ligand-ion present in great excess compared to component 1 at all places. The product is component 2 having no retention A(2)=1. The reaction is assumed reversible:

$$C1 + L \xrightarrow{K_1} C_2$$

$$C2 \xrightarrow{K_2} C1 + L$$

Each of these reactions can be characterized by half lives which are:

$$t_{1/2} = \ln 2/(K_1[L])$$
$$t_{1/2} = \ln 2/K_2$$

respectively, where [L] is the concentration of the ligand-ion, L. A comparison of half-lives to the residence time for the two components in the column will tell whether equilibrium is maintained during the migration or not. The residence times in this case will be 200 and 100 years for component 1 and 2, respectively. Three different situations are considered, the equilibrium, intermediate, and non-equilibrium cases:

$K_1[L] = K_2$ in years^{-1}	$t_{1/2}$ in years	case
1	0.693	equilibrium
0.1	6.93	intermediate
0.01	63.3	non-equilibrium

Input data:

```
100 THIS IS TEST CASE NO. 3A
200 PLO3AC
300 PLO3AE
400 1,2,1,1
500 2
```

```
 600 401
 700 100
 800 40
 900 4
1000 1.0
1100 200
1200 100000
1300 0.5
1400 1,0,1,1,1,1,0
1500 0.03
1600 2.,2.,1.,1
1700 0
1800 1
1900 0
2000 1
2100 0
2200 -1.,1
2300 1.,-1
2400 2,2
2500 0,200,196
2600 1.535
2700 0,200,196
2800 1.535
```

The two components are put on the column in equal amounts and under equal conditions.

From the plotted output in Fig. 6.3 it is seen that the two components migrate with the same velocity equal to the mean of the velocities of the individual components. This behaviour is expected because of the high reaction rates, which maintain chemical equilibrium at all times.

6.5. Test example 3B

This test example is identical to the previous one, except that the reaction rates are changed to shift the equilibrium in favour of component 2.

Input data:

```
 100 THIS IS TEST CASE NO. 3B
 200 PLO3BC
 300 PLO3BE
 400 1,1,1,1
 500 2
 600 401
 700 100
 800 40
 900 4
1000 1.0
1100 200
1200 100000
1300 0.5
1400 1,0,1,1,1,1,0
1500 0.03
1600 2.,2.,1.,1
1700 0
1800 1
1900 0
2000 1
2100 0
2200 -2.,1
2300 2.,-1
2400 2,2
2500 0,200,196
2600 1.535
2700 0,200,196
2800 1.535
```

From the plotted output in Fig. 6.4 it is seen that the relative amounts are shifted to the equilibrium ratio (1:2) and also the common migration velocity is increased in favour of component 2 compared with the previous example.

6.6. Test example 3C

This is the intermediate case.

Input data:

```
 100 THIS IS TEST CASE NO. 3C
 200 PLO3CC
 300 PLO3CE
 400 1,2,1,1
 500 2
 600 401
 700 100
 800 40
 900 4
1000 1.0
1100 280
1200 100000
1300 0.5
1400 1,0,1,1,1,1,0
1500 0.03
1600 2.,2.,1.,1
1700 0
1800 1
1900 0
2000 1
2100 0
2200 -.1,.1
2300 .1,-.1
2400 2,2
2500 0,200,196
2600 1.535
2700 0,200,196
2800 1.535
2900 210
```

From the plotted output in Fig. 6.5 it is seen that the effect is to broaden the eluate and the concentration profiles. The ini-

tially produced skewness in the concentration profiles is damped during migration. The original skewness is due to the different retention of the two components.

6.7. Test example 3D

In this test example the half-lives of the reactions is comparable to the residence time in the column.

Input data:

```
 100 THIS IS TEST CASE NO. 3D
 200 PLO3DC
 300 PLO3DE
 400 1,2,1,1
 500 2
 600 401
 700 100
 800 40
 900 4
1000 1.0
1000 260
1200 100000
1300 0.5
1400 1,0,1,1,1,1,0
1500 .03
1600 2.,2.,1.,1
1700 0
1800 1
1900 0
2000 1
2100 0
2200 -.01.,01
2300 .01,-.01
2400 2,2
2500 0,200,196
2600 1.535
2700 0,200,196
2800 1.535
```

From the plotted output in Fig. 6.6 it is seen that the compounds show peaks that move with the velocities of the individual components. Besides these peaks the components have a "tail" in front and behind the peak, respectively.

6.8. Test example 3E

The only change here compared to example 3D is that of the relative reaction rates.

Input data:

```
 100 THIS IS TEST CASE NO. 3E
 200 PLO3EC
 300 PLO3EE
 400 1,2,1,1
 500 2
 600 401
 700 100
 800 40
 900 4
1000 1.0
1100 260
1200 100000
1300 0.5
1400 1,0,1,1,1,1,0
1500 0.03
1600 2.,2.,1.,1
1700 0
1800 1
1900 0
2000 0.3
2100 0
2200 -.02,.01
2300 .02,-.01
2400 2,2
2500 0,200,196
2600 1.535
2700 0,200,196
```

It is seen from the plotted output in Fig. 6.7 that this gives rise to a change in the relative amounts of the two components, as expected.

6.9. Test case 4A and 4B

In order to test the retention subroutines, test examples 4A and 4B were constructed.

Input data:

```
 100 TEST CASE NO. 4A: A=1; V=1;
 200 AV1C
 300 AV1E
 400 1,2,1,1
 500 1
 600 401
 700 100
 800 20
 900 1
1000 1
1100 200.0
1200 100000
1300 1
1400 1,1,1,1,1,1,1
1500 0.03
1600 1.,1
1700 0
1800 1
1900 0
2000 1
2100 0
2200 0
2300 2
2400 0,205,201
2500 1.0
```

```
 100 TEST CASE NO. 4B: A=10; V=10;
 200 AV1C
 300 AV1E
 400 1,2,1,1
 500 1
 600 401
 700 100
 800 20
 900 1
1000 10.0
1100 200
1200 100000
1300 1
1400 1,1,1,1,1,1,1
1500 0.03
1600 10.,10
1700 0
1800 1
1900 0
2000 1
2100 0
2200 0
2300 2
2400 0,205,201
2500 1.0
```

The only difference between these two inputs is that 4A has V=1 and A=1, and 4B has V=10 and A=10. In Fig. 6.8 the plotted output is shown with the two eluate plots superimposed. From the eluate plots it is seen that the peak leaves the column at the same time in both cases as they must. Also it is seen that the concentration profiles are narrower in case 4B, where only one tenth of the concentration is available for dispersion.

6.10. Test example 5

In test examples 5A, 5B, and 5C the algorithm for second order reactions alone are tested. Components 1 and 2 react to give 3 and 4 and vice versa. The input for the three cases are indentical except for the concentration input. In 5A all 4 components have been put on the column in equal concentrations. In 5B only components 1 and 2 are added in equal concentrations and in 5C only components 3 and 4 are added to the column also in equal concentrations.

Input data:

```
 100 TEST EXAMPLE 5A
 200 F4C
 300 F4E
 400 0,0,1,0
 500 4
 600 401
 700 800
 800 100
 900 4
1000 5
1100 200
1200 100000
1300 .2
1400 1,1,1,1,1,1,1
1500 .1
1600 1.,1
1700 0
```

```
1800 1
1900 0
2000 2
2100 2
2200 1,2,3,4,.02
2300 2,3,1,2,.92
2400 0
2500 1,1,1,1
2600 1,1.,.5
2700 1,1.,.5
2800 1,1.,.5
2900 1,1.,.5
```

The plotted output from these three test examples are all shown in Fig. 6.9. Since all components are already in equilibrium when introduced in the column in 5A it looks like they proceed through the column as if no reactions where taking place. In 5B only component 1 and 2 are added in twice the concentration as in 5A. Here component 3 and 4 build up through the column and the same equilibrium is obtained at the end of the column where the four peaks are identical to what is seen in 5A. In 5C components 3 and 4 are added analogously to 5B. Components 1 and 2 bui'd up through the column and the same equilibrium peaks are observed at the end as expected.

6.11. Test example 6

In test examples 6A, 6B, and 6C combinations of first and second order kinetics is shown along with the effect of variation of the time step. Component 1 and 2 react to give component 3, which reacts back to give 1 and 2. In 6A the input concentration was given as component 3 only and in 6B input concentration was given as component 1 and 2 in equal concentrations.

Input data:

```
 100 TEST EXAMPLE 6A
 200 ABC6AC
 300 ABC6AE
 400 0,2,1,0
 500 3
 600 401
 700 120
 800 20
 900 1
1000 1
1100 200
1200 100000
1300 1
1400 1,1,1,1,1,1,0
1500 0.03
1600 1.,1
1700 0
1800 1
1900 0
2000 1
2100 1
2200 2,1,3,0,.4
2300 0.,0.,.4
2400 0.,0.,.4
2500 0.,0.,-.4
2600 2,2,2
2700 0,205,201
2800 0,205,201
2800 0
2900 0,205,201
3000 0
3100 0,205,201
3200 1
```

The plotted output is shown in Fig. 6.10. It is seen that equilibrium is already obtained after 20 years and the same peaks are observed in 6A and 6B as observed. A closer inspection of the

peaks reveals that they are a little skew. This can be due only to the discrete nature of the second order calculation. Application of very small timesteps, however, will remove the skewness, but the process will be very time consuming. Example 6C shows what can happen if you choose a timestep that is too large. From 6A to 6C the only change was to increase the timestep from 1 to 2. The amount to be reacted in a second order reaction is calculated as:

```
DELTAT * SR * R1 * R2 ,
```

where DELTAT is the time step, SR the second order rate constant, R1 and R2 the concentrations of the two reactants. The factors in this expression may have values that causes the amount to be reacted to be greater than what is available for reaction causing "negative" concentrations. If this happens a warning is given at the terminal. An output option (IOUT(3)) exists that sets small negative concentrations that may occur in the beginning of a calculation equal to zero.

7. HOW TO RUN COLUMN2 ON THE RISØ B7800 COMPUTER

COLUMN2 can be run either interactively or as a batch job. In both cases the input file has to be made up and saved on the disk in advance. After log-on the program is run with the following run statement:

```
Run COLUMN2; file file1 = inputfilename.
```

File 1 has been defined as a disk file titled: IFILE. However, the run statement shown will allow any input file name, which is of great practical importance. The terminal has to be a graphics terminal in order to get the output plots shown on the screen.

The alpha-numeric output of the previous run statement will depend on how the output options are set. The title is always shown on the terminal as a signal indicating that reading of the input file has begun. Errors in the input file will give standard error messages on the terminal. When the calculation is finished the terminal will show "PLEASE", which means that the output plots are ready for inspection and/or further treatment, e.g. stored in an imagefile or plotted on paper at the computer installation or on a side plotter. When run interactively there is a maximum run time of 60 processor seconds set by the computer installation at Risø. The run time depends on a number of parameters: time step, number of components, number of reaction, length of column, and the number of years (TMAX) for which the calculation is performed. If the calculation is stopped because of lack of computing time the terminal will show "INTERRUPTED BECAUSE OF TIMELIMIT" and "PLEASE" on the next line.

When COLUMN2 is run as a batch job a job-file of the type shown below is needed:

```
100 ?BEGIN JOB TEST; CLASS=0 ; CHARGE=3520001; MAXPROCTIME=600;
110 MAXIOTIME=600; PRINTLIMIT=1000;
200 RUN OBJECT/COLUMN2
210 FILE FILE1=INPUT FILENAME
220 FILE FILE6 (PRINTER)
300 ?END JOB
```

"TEST" is just a name of the job for identification purposes. There exists different classes of jobs with different limits to processor time printout, etc. The show job is of class 0 with ulimited resources, which have to be specified. "Charge" is the account number from which the costs are paid. "MAXPROCTIME" is the specification of the maximum processer-time, here 600 seconds. In the second line is specified maximum io-time in seconds and maximum print output in lines. The third line has the run statement. Line 400 defines the input file name, line 500 defines the output file to be the printer,and line 600 ends the job file. The job is started with a statement: start jobfilename.

When COLUMN2 is run as a batch job the resulting plots are stored in an image file named IMSAVE.

8. ADAPTION OF THE CODE FOR OTHER COMPUTERS

COLUMN2 is written in standard FORTRAN77 and should as such be portable to any other computer having a FORTRAN77 compiler. The program uses Risø Interactive Graphics System, RIGS (Rahbek and Hansen 1983) and an integration routine, SPLINT, from Risø Computer Library, RCL. It should be no problem to substitute SPLINT which evaluates the integral of a tabulated function in non-equidistant prints using cubic spline quadrature with some other standard integration routine.

The missing availability of RIGS on another computer may cause more serious problems. It will not be attempted here to give a complete list of the problems and the modifications needed to make COLUMN2 run the same way as on our computer. Plotting of the concentration profiles should be no problem since only simple plot statements are used. However, frames, text and storing of the plots have to be altered completely.

9. HOW TO GET THE COLUMN 2 PROGRAM

A copy of the program with listing can be obtained free of charge by sending a blank 9 track tape to:

Ole John Nielsen
Chemistry Department
Risø National Laboratory
DK 4000 Roskilde
Denmark

Also your request should contain information as to what density (6250, 1600 or 800 bpi), record length, and blocksize you want. Assistance for modifications and implementation will be given on a commercial basis.

10. CONCLUSION

On the basis of the old COLUMN program a new COLUMN2 program has been constructed and tested. The various physical and chemical processes that may influence migration have been listed. Mathematical decriptions and numerical methods have been treated in great detail. A large number of test examples with both input and output have been given. As far as the authors know, COLUMN2 presents the first attempt to include second order kinetics in a computer program for simulation of migration. The discrete nature of the calculation of second order kinetics can give rise to numerical problems. Several solutions, e.g. variable time steps to this problem could have been suggested. However, the authors found it more important to keep the program so simple that users would have a better feeling for what is taking place. It was not intended to construct a fully automatized program. The program and this manual are available on request.

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APPENDIX I

Alphabetic list of variables, parameters, identifiers, and units

A	Two-dimensional array of retention factors
AE	Retention factor for a component at the end of the column
AS	Retention factor for a component at the star of the column
C	Three-dimensional array for concentrations
CE	Two-dimensional array for effluent concentrations
CINT	Integrated concentration
CINT1	Maximum integrated sum of concentration
CIRCTI	Processor time between two concentration profiles
CLASS	Input identifier for IOUT(2); 0, 1 or 2
CONE	One-dimensional array for concentration
CONTIME	Duration time for a concentration input pulse
CT	Interpolated concentration
C0	Input concentration
C1	Three dimensional array for concentrations used during redistribution of points
D	Dispersion coefficients
DCINT	Fraction to which the summed concentrations must be removed from the column before calculation is stopped. Permanently set equal to 100000
DELTAT	Timestep
DIFD	Input identifier for different dispersion coefficients
DIFMAXC	Input identifier for different YCMAX
DIFMAXE	Input identifier for different YEMAX
DIFMINC	Input identifier for different YCMIN

DIFMINE Input identifier for different YEMIN

DIFRATE Input identifier for different S

DIFRET Input identifier for different AS and AE

HC Input identifier for IOUT(5); YES/NO

ICIN Parameter (0,1, or 2) determining the input mode of the concentrations (continuous, pulse, etc.)

IENPOI Endpoint of the input concentration

IFORM Parameter (0 or 1) determining the form of the input concentration (square or user-defined)

II Number of time steps between concentration profiles

III Number of time steps between effluent collection

IMSAVE Name of the image file for saving output plots

INPUT Input identifier for getting input

INSR Number of second order reactions

INT Input identifier for IOUT(4); YES/NO

IOLDNI Array denoting the first point inside the column in the previous calculation cycle

IOPT Array giving input options for D, A, YCMIN, YCMAX, YEMIN, YEMAX, and S

IOUT Array giving output and calculation options

IP Input identifier for IOUT(1); YES/NO

IPLCOU Counter for the number of concentration profiles plotted

ISTPOI Start point for input concentration

KNOTS Number of points in integration of a concentration profile

LIST Input identifier listing the input on the terminal

M Number of points in the calculation (must be uneven)

N Number of components

NEG	Boolean, default value, false. Can be set true using IOUT(3) = 0 causing negative concentrations to be set equal to zero
NEG	Input identifier for IOUT(3); YES/NO
NEWFIL	Boolean permanently set false to indicate that image file exists
NI	First point inside the column
NNI	Last point inside the column
OLDTI	Summed processor time
P	Length of column
PLNAC	Variable containing the name by which the concentration output plot is identified
PLNAE	Variable containing the name by which the effluent output plot is identified
P1	Number of first product component
P2	Number of second product component
PF	Input identifier for input pulses, forms and concentrations
RN	Counter for second order reactions
R1	Number of first reactant component
R2	Number of second reactant component
S	Two-dimensional array giving first order rate constants
SAVE	Input identifier for saving the input
SOR	Input identifier for second order reactions
SR	Second order rate constants
STOP	Input identifier for stoping COLUMNINPUT
T	Time
TIME	Processor time
TITLE	Input identifier for title

TMAX	Maximum time (not processor time) before the calculation is stopped
V	Velocity of the flow
VAL	Value of the integrated concentration profile
WORK	Working array for the subroutine SPLINT
X	Two-dimensional array giving position of points
XX	One-dimensional array giving position of points for the subroutine SPLINT
X1	Two-dimensional array giving position of points used in redistribution of points
YCMAX	Maximum ordinate value in the concentration plots
YCMIN	Minimum ordinate value in the concentration plots
YEMAX	Maximum ordinate value in the effluent plot
YEMIN	Minimum ordinate value in the effluent plot

Units

time:	year
length:	m
concentration:	moles m^{-3}
dispersion coefficient:	m^2 $year^{-1}$
first order rate constants:	$year^{-1}$
second order rate constants:	m^3 $moles^{-1}$ $year^{-1}$
velocity:	m $year^{-1}$

APPENDIX II: Listing of the COLUMN2 program

```
100 $RESET FREE
200 C ***************************************************************
300 C                                                                *
400 C                          PROGRAM COLUMN2                       *
500 C                                                                *
600 C            OLE JOHN NIELSEN, LARS CARLSEN, AND PETER BO        *
700 C                                                                *
800 C          CHEMISTRY DEPARTMENT, RISOE NATIONAL LABORATORY       *
900 C                                                                *
1000 C                   DK-4000 ROSKILDE, DENMARK                   *
1100 C                                                               *
1200 C                    PHONE: 2-371212 EXT. 5331                  *
1300 C                                                               *
1400 C ***************************************************************
1500 FILE  1(KIND='DISK', TITLE='IFILE.', FILETYPE=7)
1600 FILE  2(KIND='PRINTER')
1700 FILE  3(KIND='DISK',TITLE='IMSAVE.',FILETYPE=7)
1800 $INCLUDE 'RISOE/BLOCKGLOBALS/F77'
1900 $INCLUDE 'RISOE/RIGS/F77'
2000 $INCLUDE '*RISOE/RISOE/F77'
2100       DIMENSION C(3,5,801),X(5,801),CE(5,801),NI(5),NNI(5),YEMAX(5)
2200       DIMENSION P2(10),D(5),CO(5),A(5,801),YCMIN(5),YCMAX(5),YEMIN(5)
2300       DIMENSION COTIME(5),X1(5,801),C1(2,5,801)
2400       DIMENSION S(5,5),JI(5),AS(5),AE(5),SR(10),R1(10),R2(10),P1(10)
2500       DIMENSION XX(801),COME(801),WORK(2500)
2600       DIMENSION IOPT(7),IOUT(5),ISTPOI(5),IENPOI(5)
2700       DIMENSION IOLDNI(5),ICIN(5),IFORM(5)
2800       INTEGER R1,R2,P1,P2,RN
2900       LOGICAL NEG,NEWFIL
3000       CHARACTER*36 TEXT2,TEXT3,TEXT12,TEXT13
3100       CHARACTER*72 TITLE
3200       CHARACTER*6 PLNAC,PLNAE,IMSAVE
3300 C ***************************************************************
3400 C *** START TEXT ***************************************************
3500 C ***************************************************************
3600       DATA TEXT2/'CONC. PROFILES  DT=         YEARS     '/
3700       DATA TEXT3/'0              X M                    '/
3800       DATA TEXT12/'ELUATE CONC.   L=        M          '/
3900       DATA TEXT13/'0             T YEARS                '/
4000 C ***************************************************************
4100 C *** END TEXT *****************************************************
4200 C ***************************************************************
4300 C ****INITIATION OF PLOTTING DEVICES ********************************
4400 C ***************************************************************
4500       CALL RINIT
4600       CALL SIMFIL('IMSAVE',NEWFIL)
4700       NEWFIL=.FALSE.
4800       CALL SDEVI('TERM','TEK4014')
4900       CALL SDEVI('PLOT','C1012')
5000       CALL SDEVI('HARD','T4662')
5100       CALL SWINDO(0.,0.,30.,40.)
5200       CALL SMAP('TERM',1)
5300       CALL SMAP('PLOT',1)
5400       CALL SMAP('HARD',1)
5500       CALL SHEIGH('PLOT',20.)
5600       CALL SBAUD(9600)
5700       CALL SAUTO(.FALSE.)
5800 C ***************************************************************
5900 C **END INITIATION OF PLOTTING DEVICES ****************************
6000 C ***************************************************************
```

```
C *** START INPUT-DATA ***************************************************
C ************************************************************************
      READ (1,701) TITLE
  701 FORMAT (A72)
  702 FORMAT (A6)
      WRITE (6,801) TITLE
      READ(1,702) PLMAC
      READ(1,702) PLMAE
  801 FORMAT (1X, A72)
      READ (1,*) (IOUT(I), I=1,5)
      READ (1,*) N, M, P, II, III
      READ (1,*) V, TMAX, DCINT, DELTAT
      READ (1,*) (IOPT(I), I=1,7)
      IF (IOPT(1).EQ.0) GO TO 201
      READ (1,*) D(1)
      DO 301 I = 1, N
  301 D(I) = D(1)
      GO TO 202
  201 READ (1,*) (D(I), I= 1,N)
  202 CONTINUE
      IF (IOPT(2).EQ.0) GO TO 203
      READ (1,*) AS(1), AE(1)
      DO 307 I = 1, N
      AS(I)=AS(1)
      AE(I)=AE(1)
  307 CONTINUE
      GO TO 204
  203 READ(1,*) (AS(I),AE(I), I= 1,N)
  204 CONTINUE
      DO 308 I=1,N
      IF(AS(I).EQ.AE(I)) THEN
        DO 309 L=1,M
        A(I,L)=AS(I)
  309   CONTINUE
      ENDIF
  308 CONTINUE
      IF (IOPT(3).EQ.0) GO TO 205
      READ (1,*) YCMIN(1)
      DO 303 I = 1, N
  303 YCMIN(I) = YCMIN(1)
      GO TO 206
  205 READ (1,*) (YCMIN(I), I= 1,N)
  206 CONTINUE
      IF (IOPT(4).EQ.0) GO TO 207
      READ (1,*) YCMAX(1)
      DO 304 I = 1, N
  304 YCMAX(I) = YCMAX(1)
      GO TO 208
  207 READ (1,*) (YCMAX(I), I= 1,N)
  208 CONTINUE
      IF (IOPT(5).EQ.0) GO TO 209
      READ (1,*) YEMIN(1)
      DO 305 I = 1, N
  305 YEMIN(I) = YEMIN(1)
      GO TO 210
  209 READ (1,*) (YEMIN(I), I= 1,N)
  210 CONTINUE
      IF (IOPT(6).EQ.0) GO TO 211
      READ (1,*) YEMAX(1)
      DO 306 I = 1, N
```

```
12100   306 YEMAX(I) = YEMAX(1)
12200       GO TO 212
12300   211 READ (1,*) (YEMAX(I), I= 1,N)
12400   212 CONTINUE
12500       READ(1,*) INSR
12600       IF(INSR.EQ.0) GO TO 219
12700       DO 218 I=1,INSR
12800       READ(1,*) R1(I), R2(I), P1(I), P2(I), SR(I)
12900   218 CONTINUE
13000   219 CONTINUE
13100       IF (IOPT(7).EQ.0) GO TO 213
13200       READ(1,*) S(1,1)
13300       DO 310 I=1,N
13400       DO 311 L=1,N
13500       S(I,L)=S(1,1)
13600   311 CONTINUE
13700   310 CONTINUE
13800       GO TO 214
13900   213 DO 312 I=1,N
14000   312 READ(1,*) (S(I,L),L=1,N)
14100   214 CONTINUE
14200 C ***********************************************************************
14300 C *** END INPUT-DATA ********************************************************
14400 C ***********************************************************************
14500 C     INITIAL VALUES OF COUNTERS ETC.
14600 C     IJK   REGULATES THE PLOT OF FRAMES AND TEXT
14700       IJK=1
14800 C     II2 AND II1 IDENTIFIES THE CONCENTRATION ARRAYS FOR T-DT AND
14900 C     T RESPECTIVELY
15000       II1=1
15100       II2=2
15200 C     II3 CHANGES THE VALUE (1 OR 2) OF II1 AND II2
15300       II3=-1
15400 C     II4 IS COUNTER FOR CONC. PROFILE OUTPUT,COUNTING UP TO II
15500       II4=0
15600 C     II5 IS COUNTER FOR COLLECTING EFFLUENT CONC,COUNTING UP TO III
15700       II5=0
15800 C     T IS THE TIME FROM START
15900       T=0.
16000 C     II6 IS TIME COUNTER FOR EFFLUENT CONC. CE(I,II6)
16100       II6=0
16200       CINT1=0
16300       IPLCOU=0
16400       NEG=.TRUE.
16500 C ***********************************************************************
16600 C ***** START INITIAL CONCENTRATION PROFILE ***************************
16700 C ***********************************************************************
16800       READ(1,*) (ICIN(I), I=1,N)
16900       DO 313 I=1,N
17000       C0(I)=0.
17100       NI(I)=(M-1)/2
17200       NNI(I)=M
17300       DO 316 L=1,M
17400       X(I,L)=P*2.*P*L/(M-1)
17500       C(II1,I,L)=0.
17600       C(II2,I,L)=0.
17700       C(3,I,L)=0.
17800   316 CONTINUE
17900       IF (ICIN(I).EQ.0) GO TO 215
18000       IF(ICIN(I).EQ.2) GO TO 220
```

```
18100       READ(1,*) IFORM(I),COTIME(I),CO(I)
18200       IF (IFORM(I).EQ.0) GO TO 216
18300       GO TO 217
18400   216 CONTINUE
18500 C ***************************************************************************
18600 C *** IN 216 YOU CAN ENTER AN INPUT-SUBROUTINE *******************************
18700 C ***************************************************************************
18800       GO TO 217
18900   215 READ(1,*) CO(I)
19000       DO 318 L=1,(M-1)/2
19100       C(II1,I,L)=CO(I)
19200       C(II2,I,L)=CO(I)
19300   318 CONTINUE
19400       GO TO 217
19500   220 READ(1,*) IFORM(I),ISTPOI(I),IENPOI(I)
19600       IF(IFORM(I).EQ.0) GO TO 221
19700       READ(1,*) (C(II1,I,L), L=IENPOI(I),ISTPOI(I))
19800       DO 222 L=IENPOI(I),ISTPOI(I)
19900   222 C(II2,I,L)=C(II1,I,L)
20000       GO TO 217
20100   221 READ(1,*) C(II1,I,ISTPOI(I))
20200       IF (ISTPOI(I).GE.((M-1)/2)-1.AND.IE POI(I).LE.(M-1)/2) CO(I)=C(II
20300      1,I,ISTPOI(I))
20400       DO 315 L=IENPOI(I),ISTPOI(I)
20500       C(II1,I,L)=C(II1,I,ISTPOI(I))
20600       C(II2,I,L)=C(II1,I,ISTPOI(I))
20700   315 CONTINUE
20800   217 CONTINUE
20900   313 CONTINUE
21000 C ***************************************************************************
21100 C ***** END INITIAL CONCENTRATION PROFILE ************************************
21200 C ***************************************************************************
21300 C *** PRINTING OF INPUT ********************************************************
21400 C ***************************************************************************
21500       IF(IOUT(1).EQ.1) GO TO 102
21600       WRITE(2,*) TITLE
21700       WRITE(2,*) PLNAC,'  ',PLNAE
21800       WRITE(2,*) ('IOUT OF ',I,'=',IOUT(I),'  ', I=1,5)
21900       WRITE(2,*) 'NUMBER OF COMPONENTS, N=',N
22000       WRITE(2,*) 'NUMBER OF POINTS, M=',M
22100       WRITE(2,*) 'LENGTH OF COLUMN, P=',P
22200       WRITE(2,*) 'TIME STEPS BETWEEN CONCENTRATION PROFILES, II=',II
22300       WRITE(2,*) 'TIME STEPS BETWEEN EFFLUENT COLLECTION, III=',III
22400       WRITE(2,*) 'VELOCITY, V=',V
22500       WRITE(2,*) 'MAXIMUN TIME, TMAX=',TMAX
22600       WRITE(2,*) 'DCINT=',DCINT
22700       WRITE(2,*) 'DELTAT=',DELTAT
22800       WRITE(2,*) ('IOPT OF ',I,' = ',IOPT(I),'  ', I=1,7)
22900       WRITE(2,*) ('D OF ',I,' = ',D(I),'  ', I=1,N)
23000       WRITE(2,*) ('AS OF ',I,' = ',AS(I),'  AE OF ',I,' = ',AE(I),'  ',
23100      1=1,N)
23200       WRITE(2,*) ('YCMIN OF ',I,' = ',YCMIN(I),'  YCMAX OF ',I,' = ',YC
23300      1AX(I),'  ', I=1,N)
23400       WRITE(2,*) ('YEMIN OF ',I,' = ',YEMIN(I),'  YEMAX OF ',I,' = ',YE
23500      1AX(I),'  ', I=1,N)
23600       WRITE(2,*) 'NUMBER OF SECOND ORDER REACTIONS, INSR=',INSR
23700       IF(INSR.EQ.0) GO TO 106
23800       DO 107 I=1,INSR,1
23900       WRITE(2,*) ('REACTION: ',I,'  ',R1(I),'+',R2(I),' GIVES ',P1(I),'
24000      1',P2(I),'  RATE CONSTANT=',SR(I),'    ',I=1,INSR)
```

```
24100   107  CONTINUE
24200   106  DO 108 I=1,N,1
24300        WRITE(2,*) 'FIRST ORDER RATE CONSTANTS: ',(L,' TO ',I,'=',S(I,L),
24400       1L=1,N)
24500   108  CONTINUE
24600        WRITE(2,*) ('ICIN OF ',I,' = ',ICIN(I),'  ', I=1,N)
24700        WRITE(2,*) ('FORM OF ',I,' = ',IFORM(I),'  ', I=1,N)
24800        DO 103 I=1,N
24900        IF(ICIN(I).EQ.0) GO TO 104
25000        IF(ICIN(I).EQ.2) GO TO 109
25100        WRITE(2,*) 'COMPONENT: ',I,'  COTIME= ',COTIME(I),'  CO= ',CO(I)
25200   103  CONTINUE
25300        GO TO 105
25400   104  WRITE(2,*) 'CONTINOUS INPUT OF ',I,' CONCENTRATION= ',CO(I)
25500        GO TO 103
25600   109  WRITE(2,*) 'COMPONENT: ',I,'  START= ',ISTPOI(I),' END= ',IENPOI(
25700       1),'  "CONCENTRATION"= ',C(II1,I,ISTPOI(I))
25800        GO TO 103
25900   105  CONTINUE
26000 C ***************************************************************
26100 C *** END PRINTING OF INPUT *********************************************
26200 C ***************************************************************
26300   102  CONTINUE
26400        GO TO 100
26500   101  CONTINUE
26600   502  FORMAT(3E15.4,2I10)
26700        CALL REDISP(X,C,X1,C1,II2,I,M,P)
26800        DO 503 L=1,M,1
26900        X(I,L)=X1(I,L)
27000        C(II2,I,L)=C1(II2,I,L)
27100        C(II1,I,L)=C1(II2,I,L)
27200   503  CONTINUE
27300        WRITE(6,500) T
27400   500  FORMAT(1HO,20X,'REDISTRIBUTION AT T=',E15.4/1X)
27500        II3=-II3
27600        II1=II1+II3
27700        II2=II2-II3
27800        NI(I)=(M-1)/2
27900        NNI(I)=M
28000 C      FIND THE BOUNDARY OF THE COLUM
28100   100  DO 3 I=1,N,1
28200        IOLDNI(I)=NI(I)
28300   4    J=NI(I)
28400        IF(X(I,J).GE.0.) NI(I)=NI(I)-1
28500        IF(NI(I).EQ.0) GO TO 101
28600        IF(X(I,J).GE.0.) GO TO 4
28700        JI(I)=NI(I)+1
28800   5    J=NNI(I)
28900        IF(X(I,J).GE.P) NNI(I)=NNI(I)-1
29000        IF(X(I,J).GE.P) GO TO 5
29100   3    CONTINUE
29200 C      CHANGE THE CONCENTRATION ARRAYS
29300        II3=-II3
29400        II1=II1+II3
29500        II2=II2-II3
29600 C      CALC.RETENTION FACTORS
29700        CALL RETSUB(II2,X,C,A,N,M,P,AS,AE)
29800 C ***************************************************************
29900 C *** START BOUNDARY CONDITION AT X=0 ***************************
30000 C ***************************************************************
```

```
30100       DO 66 I=1,N,1
30200       IF (ICIN(I).EQ.0) GO TO 66
30300       IF(ICIN(I).EQ.2) GO TO 319
30400       IF(T.LE.COTIME(I)) THEN
30500       DO 67 L=NI(I)+1,IOLDNI(I)+1,1
30600       C(II1,I,L)=CO(I)
30700       C(II2,I,L)=CO(I)
30800  67   CONTINUE
30900       ELSE
31000       ENDIF
31100       IF(T.GT.COTIME(I)) CO(I)=0.
31200       GO TO 66
31300  319  IF(IENPOI(I).GT.(M-1)/2) GO TO 66
31400       IF(T.GT.((ISTPOI(I)-IENPOI(I)+1)/((V*M)/(2*P)))) CO(I)=0.
31500 66    CONTINUE
31600 C ********************************************************************
31700 C *** END BOUNDARY CONDITION AT X=0 ***********************************
31800 C ********************************************** **********************
31900       DO 6 I=1,N,1
32000       JJ=1
32100       J=NI(I)
32200       IF(X(I,J+1).LT.P/(500.*M)) JJ=0
32300       IF(JJ.EQ.0)  C(II1,I,J+1)=CO(I)
32400       IF(JJ.EQ.0) GO TO 7
32500       H=2.*X(I,J+1)/X(I,J+2)
32600       C(II1,I,J+1)=C(II2,I,J+1)+D(I)*DELTAT*(H*(C(II2,I,J+2)-C(II2,I,J+
32700      1))-(2.-H)*(C(II2,I,J+1)-CO(I)))/(A(I,J+1)*X(I,J+1)*(X(I,J+2)-X(I,
32800      2+1)))
32900 C ********************************************************************
33000 C ***** START REACTIONS AT BEGINNING OF COLUMN ************************
33100 C ********************************************************************
33200 C *** FIRST ORDER REACTIONS ************************************************
33300 C ********************************************************************
33400       DO 70 JK=1,N,1
33500       IF(S(I,JK).EQ.0) GO TO 70
33600       IF(X(JK,JI(JK)).LT.P/(500.*M)) JI(JK)=JI(JK)+1
33700       CT=CO(JK)+X(I,J+1)*(C(II2,JK,JI(JK))-CO(JK))/X(JK,JI(JK))
33800       C(II1,I,J+1)=C(II1,I,J+1)+DELTAT*S(I,JK)*CT/A(I,J+1)
33900 70    CONTINUE
34000 7     CONTINUE
34100 6     CONTINUE
34200 C ********************************************************************
34300 C *** SECOND ORDER REACTIONS **********************************************
34400 C ********************************************************************
34500       IF(INSR.EQ.0) GO TO 725
34600       DO 723 I=1,N,1
34700       DO 724 JK=1,N,1
34800       IF(X(JK,JI(JK)).LT.P/(500.*M)) JI(JK)=JI(JK)+1
34900  724  CONTINUE
35000       DO 71 RN=1,INSR,1
35100       IF(I.EQ.R1(RN)) GO TO 721
35200       GO TO 72
35300  721  CT=CO(R2(RN))+X(I,J+1)*(C(II2,R2(RN),JI(R2(RN)))-CO(R2(RN)))/X(R2
35400      1RN),JI(R2(RN)))
35500       C(3,I,J+1)=C(3,I,J+1)-DELTAT*SR(RN)*CT*C(II2,I,J+1)/A(I,J+1)*.
35600      15
35700       C(3,R2(RN),J+1)=C(3,R2(RN),J+1)-DELTAT*SR(RN)*CT*C(II2,I,J+1)/
35800      1A(R2(RN),J+1)*.5
35900       C(3,P1(RN),J+1)=C(3,P1(RN),J+1)+DELTAT*SR(RN)*CT*C(II2,I,J+1)/
36000      1A(P1(RN),J+1)*.5
```

```
36100       IF(P2(RN).EQ.0) GO TO 71
36200       C(3,P2(RN),J+1)=C(3,P2(RN),J+1)+DELTAT*SR(RN)*CT*C(II2,I,J+1)/
36300      1A(P2(RN),J+1)*.5
36400       GO TO 71
36500  72   IF(I.EQ.R2(RN)) GO TO 722
36600       GO TO 71
36700  722  CT=C0(R1(RN))+X(I,J+1)*(C(II2,R1(RN),JI(R1(RN)))-C0(R1(RN)))/X(R1(
36800      1RN),JI(R1(RN)))
36900       C(3,I,J+1)=C(3,I,J+1)-DELTAT*SR(RN)*CT*C(II2,I,J+1)/A(I,J+1)*.
37000      15
37100       C(3,R1(RN),J+1)=C(3,R1(RN),J+1)-DELTAT*SR(RN)*CT*C(II2,I,J+1)/
37200      1A(R1(RN),J+1)*.5
37300       C(3,P1(RN),J+1)=C(3,P1(RN),J+1)+DELTAT*SR(RN)*CT*C(II2,I,J+1)/
37400      1A(P1(RN),J+1)*.5
37500       IF(P2(RN).EQ.0) GO TO 71
37600       C(3,P2(RN),J+1)=C(3,P2(RN),J+1)+DELTAT*SR(RN)*CT*C(II2,I,J+1)/
37700      1A(P2(RN),J+1)*.5
37800  71   CONTINUE
37900  723  CONTINUE
38000  725  CONTINUE
38100       DO 726 I=1,N,1
38200       C(II1,I,J+1)=C(II1,I,J+1)+C(3,I,J+1)
38300  726  CONTINUE
38400 C ***************************************************************
38500 C *** END REACTIONS  ************************************************
38600 C ***************************************************************
38700 C     INTEGRATION 0<X<P
38800       DO 80 I=1,N,1
38900       DO 880 J=1,N,1
39000 880   JI(J)=NI(J)-1
39100       DO 90 L=NI(I)+2,NNI(I)+1,1
39200       IF((X(I,L)-X(I,L-1))*(X(I,L+1)-X(I,L)).LE.D(I)*DELTAT/(0.5*A(I,L)
39300      1) GO TO 101
39400       H=2.*(X(I,L)-X(I,L-1))/(X(I,L+1)-X(I,L-1))
39500       H1=D(I)*DELTAT/(A(I,L)*(X(I,L+1)-X(I,L))*(X(I,L)-X(I,L-1)))
39600       C(II1,I,L)=C(II2,I,L)+H1*(H*(C(II2,I,L+1)-C(II2,I,L))-(2.-H)*(C(I
39700      12,I,L)-C(II2,I,L-1)))
39800    90 CONTINUE
39900    80 CONTINUE
40000 C ***************************************************************
40100 C ***** START REACSTIONS INSIDE THE COLUMN ************************
40200 C ***************************************************************
40300 C *** FIRST ORDER REACTIONS ***************************************
40400 C ***************************************************************
40500       DO 8 I=1,N,1
40600       DO 88 J=1,N,1
40700 88    JI(J)=NI(J)-1
40800       DO 9 L=NI(I)+2,NNI(I)+1,1
40900       DO 99 J=1,N,1
41000       IF(S(I,J).EQ.0) GO TO 99
41100 87    CONTINUE
41200       IF(X(J,JI(J)).LE.X(I,L)) GO TO 85
41300       CT=C(II2,J,JI(J)-1)+(X(I,L)-X(J,JI(J)-1))*(C(II2,J,JI(J))-C(II2,J
41400      1JI(J)-1))/(X(J,JI(J))-X(J,JI(J)-1))
41500       C(II1,I,L)=C(II1,I,L)+DELTAT*S(I,J)*CT/A(I,L)
41600       GO TO 86
41700 85    JI(J)=JI(J)+1
41800       IF(JI(J).EQ.M+1)  GO TO 101
41900       GO TO 87
42000 86    CONTINUE
```

```
42100 99     CONTINUE
42200 9      CONTINUE
42300 8      CONTINUE
42400 C ***********************************************************************
42500 C *** SECOND ORDER REACTIONS ************************************************
42600 C ***********************************************************************
42700        IF(INSR.EQ.0) GO TO 873
42800        DO 862 I=1,N,1
42900        DO 863 L=NI(I)+2,NNI(I)+1,1
43000        DO 865 IF=1,N,1
43100  872   CONTINUE
43200        IF(X(IF,JI(IF)).LE.X(I,L)) GO TO 850
43300  866   CONTINUE
43400        IF(LESS.EQ.1) GO TO 867
43500        IF(X(IF,JI(IF)).GE.X(I,L)) GO TO 864
43600        GO TO 867
43700  850   JI(IF)=JI(IF)+1
43800        LESS=1
43900        GO TO 872
44000  864   JI(IF)=JI(IF)-1
44100        GO TO 866
44200  867   LESS=0
44300  865   CONTINUE
44400        DO 73 RN=1,INSR,1
44500        IF(I.EQ.R1(RN)) GO TO 870
44600        GO TO 74
44700  870   CONTINUE
44800        CT=C(II2,R2(RN),JI(R2(RN))-1)+(X(I,L)-X(R2(RN),JI(R2(RN))-1))*(C(
44900       1I2,R2(RN),JI(R2(RN)))-C(II2,R2(RN),JI(R2(RN))-1))/(X(R2(RN),JI(R2
45000       2RN)))-X(R2(RN),JI(R2(RN))-1))
45100        C(3,I,L)=C(3,I,L)-DELTAT*SR(RN)*CT*C(II2,I,L)/A(I,L)*.5
45200        C(3,R2(RN),JI(R2(RN)))=C(3,R2(RN),JI(R2(RN)))-DELTAT*SR(RN)*CT
45300       1*C(II2,I,L)/A(R2(RN),JI(R2(RN)))*.5
45400        C(3,P1(RN),JI(P1(RN)))=C(3,P1(RN),JI(P1(RN)))+DELTAT*SR(RN)*CT
45500       1*C(II2,I,L)/A(P1(RN),JI(P1(RN)))*.5
45600        IF(P2(RN).EQ.0) GO TO 74
45700        C(3,P2(RN),JI(P2(RN)))=C(3,P2(RN),JI(P2(RN)))+DELTAT*SR(RN)*CT
45800       1*C(II2,I,L)/A(P2(RN),JI(P2(RN)))*.5
45900        GO TO 73
46000   74   IF(I.EQ.R2(RN)) GO TO 871
46100        GO TO 73
46200  871   CONTINUE
46300        CT=C(II2,R1(RN),JI(R1(RN))-1)+(X(I,L)-X(R1(RN),JI(R1(RN))-1))*(C
46400       1I2,R1(RN),JI(R1(RN)))-C(II2,R1(RN),JI(R1(RN))-1))/(X(R1(RN),JI(R
46500       2RN)))-X(R1(RN),JI(R1(RN))-1))
46600        C(3,I,L)=C(3,I,L)-DELTAT*SR(RN)*CT*C(II2,I,L)/A(I,L)*.5
46700        C(3,R1(RN),JI(R1(RN)))=C(3,R1(RN),JI(R1(RN)))-DELTAT*SR(RN)*CT
46800       1*C(II2,I,L)/A(R1(RN),JI(R1(RN)))*.5
46900        C(3,P1(RN),JI(P1(RN)))=C(3,P1(RN),JI(P1(RN)))+DELTAT*SR(RN)*CT
47000       1*C(II2,I,L)/A(P1(RN),JI(P1(RN)))*.5
47100        IF(P2(RN).EQ.0) GO TO 73
47200        C(3,P2(RN),JI(P2(RN)))=C(3,P2(RN),JI(P2(RN)))+DELTAT*SR(RN)*CT
47300       1*C(II2,I,L)/A(P2(RN),JI(P2(RN)))*.5
47400  73    CONTINUE
47500  863   CONTINUE
47600  862   CONTINUE
47700  873   CONTINUE
47800        DO 874 I=1,N,1
47900        DO 875 L=1,M,1
48000        C(II1,I,L)=C(II1,I,L)+C(3,I,L)
```

```
48100       C(3,I,L)=0.
48200   875 CONTINUE
48300   874 CONTINUE
48400 C ***********************************************************************
48500 C *** END REACTIONS  ******************************************************
48600 C ***********************************************************************
48700 C *** START BOUNDARY CONDITION AT X=P ***********************************
48800 C ***********************************************************************
48900       DO 10 I=1,N,1
49000       J=NNI(I)
49100       H=(X(I,J+2)-X(I,J+1))/(P-X(I,J))
49200       H1=H*(P-X(I,J+1))/(X(I,J)-X(I,J-1))
49300       C(II1,I,J+2)=C(II1,I,J+1)-H*(C(II1,I,J+1)-C(II1,I,J))+H1*(C(II1,I.
49400      1J)-C(II1,I,J-1))
49500   10  CONTINUE
49600 C ***********************************************************************
49700 C *** END BOUNDARY CONDITION AT X=P ************************************
49800 C ***********************************************************************
49900 C     UPDATING TIME,COUNTERS AND POSITION
50000       T=T+DELTAT
50100       II4=II4+1
50200       II5=II5+1
50300       DO 11 I=1,N,1
50400       DO 12 L=1,M,1
50500       X(I,L)=X(I,L)+V*DELTAT/A(I,L)
50600   12  CONTINUE
50700   11  CONTINUE
50800 C     COLLECTING DATA
50900       IF(II5.NE.III) GO TO 13
51000       II6=II6+1
51100       II5=0
51200       DO 14 I=1,N,1
51300   15  J=NNI(I)
51400       IF(X(I,J).GE.P) NNI(I)=NNI(I)-1
51500       IF(X(I,J).GE.P) GO TO 15
51600       J=NNI(I)
51700       IF(J.GT.801.OR.J.LT.0) WRITE(6,*) "J= ",J
51800       CE(I,II6)=C(II1,I,J)+(P-X(I,J))*(C(II1,I,J+1)-C(II1,I,J))/(X(I,J+
51900      1)-X(I,J))
52000   14  CONTINUE
52100   13  CONTINUE
52200       IF(II4.NE.II) GO TO 163
52300       CINT=0
52400 C     INTEGRAL OF EACH COMPONENT IS CALCULATED IF DESIRED
52500       IF(IOUT(4).EQ.1) GO TO 24
52600       DO 16  I=1,N
52700       M1=1
52800       M2=M
52900       DO 17  L=1,M,1
53000       IF(X(I,L).LT.0) M1=L
53100       IF(X(I,L).GE.P) GO TO 19
53200   17  CONTINUE
53300    19 M2=L
53400       KNOTS=M2-M1-1
53500       DO 18  L=M1+1,M2-1,1
53600       XX(L-M1)=X(I,L)
53700       CONE(L-M1)=C(II1,I,L)
53800   18  CONTINUE
53900       CALL SPLINT(KNOTS,XX,CONE,WORK,VAL)
54000       WRITE(6,703) I,VAL
```

```
54100  703  FORMAT(' INTEGRAL OF COMPONENT ',I2,' = ',E10.3)
54200       CINT=CINT+VAL
54300  16   CONTINUE
54400       IF(CINT.GT.CINT1)CINT1=CINT
54500       IF(CINT.LT.CINT1/DCINT)TMAX=T
54600       WRITE(6,704) CINT,CINT1,CINT1/DCINT
54700  704  FORMAT(' CINT= ',E10.3,'  CINT1= ',E10.3,'  CINT1/DCINT= ',E10.3)
54800       WRITE(6,705) T
54900  705  FORMAT(' TIME= ',E10.2,' YEARS')
55000  24   CONTINUE
55100       CIRCTI=T-OLDTI
55200       OLDTI=T
55300       II4=0
55400       GO TO 399
55500  C    REARRANGEMENT OF X-VALUES
55600  163  DO 160 I=1,N,1
55700       IF(X(I,1).GE.-2.*P/(M-1)-V*DELTAT/A(I,1)) GO TO 161
55800  160  CONTINUE
55900       GO TO 167
56000  161  DO 167 I=1,N,1
56100  162  J=NNI(I)
56200       IF(X(I,J).GE.P) NNI(I)=NNI(I)-1
56300       IF(X(I,J).GE.P) GO TO 162
56400       J=NNI(I)+2
56500       DO 166 JJ=1,M,1
56600       IF(JJ.GT.J) GO TO 164
56700       IF(X(I,J+1-JJ).LE.0.) GO TO 164
56800       X(I,M+1-JJ)=X(I,J+1-JJ)
56900       C(II1,I,M+1-JJ)=C(II1,I,J+1-JJ)
57000       C(II2,I,M+1-JJ)=C(II2,I,J+1-JJ)
57100       GO TO 165
57200  164  X(I,M+1-JJ)=X(I,M+1-JJ+1)-2.*P/(M-1)
57300       C(II1,I,M+1-JJ)=C(II1,I,M+1-JJ+1)
57400       C(II2,I,M+1-JJ)=C(II2,I,M+1-JJ+1)
57500  165  CONTINUE
57600  166  CONTINUE
57700       NNI(I)=M
57800       NI(I)=M
57900       WRITE(6,504) T
58000  504  FORMAT(1H0,20X,'REARRANGEMENT OF X-AXES AT T=',E15.4/1X)
58100  167  CONTINUE
58200  C    CHECK FOR NEGATIVE CONCENTRATIONS
58300       DO 170 I=1,N,1
58400       DO 171 L=1,M,1
58500       IF(C(II1,I,L).LT.0.AND.(X(I,L).GE.0.AND.X(I,L).LE.P)) THEN
58600       IF(.NOT.NEG) GO TO 172
58700       WRITE(6,*) 'NEGATIVE CONCENTRATION OF COMPONENT ',I,' AT POINT ',
58800      1,' AT TIME ',T,' AT ',X(I,L),' M'
58900       WRITE(6,*) 'C WAS ',C(II1,I,L)
59000       NEG=.FALSE.
59100  172  IF(IOUT(3).EQ.0) C(II1,I,L)=0
59200       ENDIF
59300  171  CONTINUE
59400  170  CONTINUE
59500  C    CHECK IF COMPUTING-TIME IS GETTING TOO CLOSE TO LIMIT
59600       IF(IOUT(2).EQ.2.AND.CIRCTI.GT.57.-TIME('PROCESSOR').AND.TIME('PRC
59700      1ESSOR').GE.54.) THEN
59800       IF(IOUT(2).EQ.2) WRITE(6,*) ' INTERRUPTED BECAUSE OF TIMELIMIT !'
59900       GO TO 406
60000       ENDIF
```

```
      IF(IOUT(2).EQ.1.AND.CIRCTI.GT.258.-TIME('PROCESSOR').AND.TIME('PR
     1CESSOR').GE.285.) THEN
      WRITE(6,*) ' INTERRUPTED BECAUSE OF TIMELIMIT !'
      GO TO 406
      ENDIF
C     NEW INTEGRATION STEP OR FINISH CALCULATION
      IF(T.GE.TMAX) GO TO 406
      GO TO 100
C $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C $$$ START PLOT CONCENTRATION PROFILES $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
  399 CONTINUE
      CALL SWINDO(-2.,6.,24.,22.+10.*(REAL(N)-1.))
      T1=II*DELTAT
      IPLCOU=IPLCOU+1
      IF(IPLCOU.GT.1) GO TO 412
      DO 413 I=1,N,1
      CALL PFRAME(3.5,10.*REAL(I),23.5,10.+10.*REAL(I),2.,1.,0)
  413 CONTINUE
      CALL BRKIM
      CALL PTEXT(TITLE,0.,11.+10.*REAL(N),0.6)
      CALL BRKIM
      DO 414 I=N,1,-1
      CALL PREALE(YCMIN(I),8,2,-2.,0.2+10.*REAL(I),0.6)
      CALL PREALE(YCMAX(I),8,2,-2.,9.2+10.*REAL(I),0.6)
  414 CONTINUE
      CALL PTEXT(TEXT2,3.5,8.,0.6)
      CALL PTEXT(PLNAC,3.5,7.,.6)
      CALL PREALF(T1,7,1,14.9,8.0,0.6)
      CALL PTEXT(TEXT3,3.5,9.2,0.6)
      CALL PREALF(P,6,1,19.9,9.2,0.6)
      CALL BRKIM
      PX=23.5
      PY=10.
      CALL PLOT(PX,PY,1)
  412 CALL SORIGO(3.5,0.)
      J=0
      DO 401 I=1,N,1
      IF(YCMAX(I).LT.0.) GO TO 407
      J=J+1
      CALL SORIGO(0.,10.)
      IF(IPLCOU.GT.1) GO TO 440
      CALL PLOT(0.,0.,1)
      PX=0.
      PY=0.
  440 J=NNI(I)
      IF(X(I,J).GE.P) NNI(I)=NNI(I)-1
      IF(X(I,J).GE.P) GO TO 440
      PX=X(I,J)*20./P
      PY=YCMIN(I)+(C(II1,I,J)-YCMIN(I))*10./(YCMAX(I)-YCMIN(I))
      CALL PLOT(PX,PY,1)
      DO 405 JJ=1,M,1
      PX=X(I,J-JJ)*20./?
      IF(PX.LT.0.) GO TO 450
      PY=YCMIN(I)+(C(II1,I,J-JJ)-YCMIN(I))*10./(YCMAX(I)-YCMIN(I))
      CALL PLOT(PX,PY,0)
  405 CONTINUE
  450 CONTINUE
  407 CONTINUE
  401 CONTINUE
```

```
66100        IJK=0
66200        GO TO 460
66300 408    PY=-10.*N
66400        CALL SORIGO(0.,PY)
66500        DO 409 I=1,N,1
66600        IF(YCMAX(I).LT.0.) GO TO 410
66700        CALL SORIGO(0.,10.)
66800 441    J=NNI(I)
66900        IF(X(I,J).GE.P) NNI(I)=NNI(I)-1
67000        IF(X(I,J).GE.P) GO TO 441
67100        PX=X(I,J)*20./P
67200        PY=YCMIN(I)+(C(II1,I,J)-YCMIN(I))*10./(YCMAX(I)-YCMIN(I))
67300        CALL PLOT(PX,PY,1)
67400        DO 411 JJ=1,M,1
67500        PX=X(I,J-JJ)*20./P
67600        IF(PX.LT.0.) GO TO 451
67700        PY=YCMIN(I)+(C(II1,I,J-JJ)-YCMIN(I))*10./(YCMAX(I)-YCMIN(I))
67800        CALL PLOT(PX,PY,0)
67900 411    CONTINUE
68000 451    CONTINUE
68100 410    CONTINUE
68200 409    CONTINUE
68300 C
68400 C $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
68500 C $$$ END PLOT CONCENTRATION PROFILES $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
68600 C $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
68700 460    CONTINUE
68800        CALL SORIGO(-3.5,-10.*N)
68900        GO TO 163
69000 406    IF(IOUT(2).EQ.2) CALL IMHAND('PLEASE')
69100        IF(IOUT(2).EQ.2) CALL CLEARS
69200        IF(IOUT(2).EQ.1.OR.IOUT(2).EQ.0) THEN
69300        READ(3,9999)IDUMMY
69400 9999   FORMAT(A6)
69500 C      THIS READ WILL WAIT UNTIL FILE3 (THE IMAGEFILE) IS AVAILABLE.
69600        CLOSE(3)
69700        CALL SAVEIM(PLNAC)
69800        IF(IOUT(5).EQ.0) CALL SHOWIM('PLOTTER')
69900        ENDIF
70000        CALL EMPTIM
70100        CONTINUE
70200 C £££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££
70300 C £££ START PLOT EFFLUENT CONCENTRATION £££££££££££££££££££££££££
70400 C £££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££
70500        DO 608 I=1,N,1
70600        CALL PFRAME(3.5,10.*REAL(I),23.5,10.+10.*REAL(I),2.,1.,0)
70700  608   CONTINUE
70800        CALL BRKIM
70900        DO 609 I=N,1,-1
71000        CALL PREALE(YCMIN(I),8,2,-2.,0.2+10.*REAL(I),0.6)
71100        CALL PREALE(YCMAX(I),8,2,-2.,9.2+10.*REAL(I),0.6)
71200  609   CONTINUE
71300        CALL PTEXT(TEXT12,3.5,8.0,0.6)
71400        CALL PTEXT(PLNAE,3.5,7.,.6)
71500        CALL PREALF(P,6,1,13.7,8.0,0.6)
71600        CALL PTEXT(TEXT13,3.5,9.2,0.6)
71700        T1=II6*DELTAT*III
71800        CALL PREALF(T1,7,1,19.3,9.2,0.6)
71900        CALL BRKIM
72000        PX=23.5
```

```
72100       PY=10.
72200       CALL PLOT(PX,PY,1)
72300       CALL SORIGO(3.5,0.)
72400       J=0
72500       DO 601 I=1,N,1
72600       IF(YEMAX(I).LT.0.) GO TO 607
72700       J=J+1
72800       CALL SORIGO(0.,10.)
72900       PX=20.
73000       PY=YEMIN(I)+(CE(I,II6)-YEMIN(I))*10./(YEMAX(I)-YEMIN(I))
73100       CALL PLOT(PX,PY,1)
73200       DO 605 JJ=1,II6-1,1
73300       PX=20.*(II6-JJ)/II6
73400       PY=YEMIN(I)+(CE(I,II6-JJ)-YEMIN(I))*10./(YEMAX(I)-YEMIN(I))
73500       CALL PLOT(PX,PY,0)
73600 605   CONTINUE
73700 607   CONTINUE
73800 601   CONTINUE
73900 C £££££££££££££££££££££££££££££££££££££££££££££££££££££££££££££
74000 C £END PLOT EFFLUENT CONCENTRATION £££££££££££££££££££££££££
74100 C £££££££££££££££££££££££££££££££££££££££££££££££££££££££££
74200       CALL SORIGO(-3.5,-10.*N)
74300       IF(IOUT(2).EQ.2) CALL IMHAND('PLEASE')
74400       IF(IOUT(2).EQ.2) CALL CLEARS
74500       IF(IOUT(2).EQ.1.OR.IOUT(2).EQ.0) CALL SAVEIM(PLNAE)
74600       STOP
74700       CALL RTERM
74800       END
74900 C &&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&
75000 C &&& SUBROUTINES FOLLOW &&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&
75100 C &&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&
75200 C
75300       SUBROUTINE REDISP(X,C,X1,C1,II,I,M,P)
75400       DIMENSION X(5,801),X1(5,801),C(2,5,801),C1(2,5,801),R(4860)
75500       X1(I,1)=X(I,1)
75600       DO 1 L=2,M,1
75700       X1(I,L)=X1(I,L-1)+2*P/(M-1)
75800       IF(X1(I,L).GT.X(I,M)) C1(II,I,L)=C(II,I,M)
75900 1     CONTINUE
76000       E=0.000001
76100       DO 2 L=1,M,1
76200       R(2*L-1)=X(I,L)
76300       R(2*L)=C(II,I,L)
76400 2     CONTINUE
76500 3     R(4*M+1)=0.
76600       R(5*M)=0.
76700       D=4*(2.-SQRT(3.))
76800       DO 6 L=1,M-1,1
76900 4     R(3*M+L)=(R(2*L+2)-R(2*L))/(R(2*L+1)-R(2*L-1))
77000       R(2*M+L)=R(2*L+1)-R(2*L-1)
77100       IF(L.EQ.1) GO TO 5
77200       R(4*M+L)=(2*(R(3*M+L)-R(3*M+L-1))/(R(2*M+L-1)+R(2*M+L)))
77300       R(5*M+L)=3.*R(4*M+L)/2.
77400 5     CONTINUE
77500 6     CONTINUE
77600 7     EE=0.
77700       DO 10 L=2,M,1
77800       LL=4*M+L
77900       B=R(LL+1)
78000       BB=((R(LL+1)-R(LL-1))/(1.+R(LL-2*M)/R(LL-2*M-1))-B)/2.
```

```
78100        B=D*(BB-R(LL)+R(LL+M))
78200        BB=SQRT(B*B)
78300        IF(BB.GT.EE) EE=BB
78400 10     R(LL)=R(LL)+B
78500        IF(E.LE.EE) GO TO 7
78600        DO 15 L=1,M-1,1
78700        LL=4*M+L
78800 15     R(LL-2*M)=(R(LL+1)-R(LL))/R(LL-2*M)
78900        DO 30 L=1,M,1
79000        IF(X1(I,L).GT.X(I,M)) GO TO 22
79100 23     CONTINUE
79200        Z=X1(I,L)
79300        DO 20 LL=1,M-1,1
79400        Q=Z-R(2*LL-1)
79500        Q1=Z-R(2*LL+1)
79600        IF(Q.GE.0..AND.Q1.LT.0.) GO TO 21
79700        IF(LL.EQ.M-1.AND.Q1.EQ.0.) GO TO 21
79800 20     CONTINUE
79900        GO TO 22
80000 21     D=R(4*M+LL)+Q*R(2*M+LL)
80100        D=(R(4*M+LL)+R(4*M+LL+1)+D)/6.
80200        D=R(2*LL)+Q*R(3*M+LL)+Q*Q1*D
80300        C1(II,I,L)=D
80400        IF(D.LE.0.) C1(II,I,L)=0.
80500 22     CONTINUE
80600 30     CONTINUE
80700        RETURN
80800        END
80900 C
81000        SUBROUTINE RETSUB(I,X,C,A,N,M,P,AS,AE)
81100        DIMENSION AS(5),AE(5),X(5,801),C(2,5,801),A(5,801)
81200        DO 1 J=1,N,1
81300        DO 2 L=1,M,1
81400        A(J,L)=AS(J)+(AE(J)-AS(J))*X(J,L)/P
81500        IF(X(J,L).LE.0.) A(J,L)=AS(J)
81600        IF(X(J L).GT.P) A(J,L)=AE(J)
81700 2      CONTINUE
81800 1      CONTINUE
81900        RETURN
82000        END
82100 $RESET LIST
£
```

APPENDIX III: Listing of the COLUMNINPUT program

```
100
200 BEGIN
300   FILE SCREEN(KIND=REMOTE,MYUSE=OUT,MAXRECSIZE=90,UNITS=1),
400       KEYBOARD(KIND=REMOTE,MAXRECSIZE=90,UNITS=1,MYUSE=IN);
500   FILE INP(KIND=DISK,FILETYPE=7);
600   FILE OUT(KIND=DISK,MAXRECSIZE=14,BLOCKSIZE=420,AREASIZE=1080,
700       NEWFILE=TRUE);
800   BOOLEAN REMOTEINPUT,INPUTFINISHED,FILEFINISHED,REMOTEJOB,INPUTPRINT,
900         NEGCON,INTEGRATION,HARDPLOT;
1000   STRING PLNAC,PLNAE,TITLE,INPUTTITLE,OUTPUTTITLE;
1100   POINTER PT,PC;
1200   ALPHA ARRAY TITLEAR,CARD[0:70];
1300   INTEGER N,M,P,III,II,INSR,I,L,J;
1400   REAL TMAX,V,DCINT,DELTAT;
1500   INTEGER ARRAY IOPT[1:7],IOUT,ISTPOI,IENPOI,ICIN,IPOHM[1:5],R1,R2,P1,
1600         P2[1:10];
1700   REAL ARRAY D,AE,AS,YCMIN,YCMAX,YEMIN,YEMAX[1:5],SR[1:10],S[1:5,1:5],
1800       C[1:5,1:801],CO,COTIME[1:5];
1900
2000   PROCEDURE PRINT(OUT);
2100   FILE OUT;
2200     BEGIN
2300       WRITE(OUT,<A*>,LENGTH(TITLE),TITLE);
2400       WRITE(OUT,<A6>,PLNAC);
2500       WRITE(OUT,<A6>,PLNAE);
2600       WRITE(OUT,<4(I1,","),I1>,FOR I:=1 STEP 1 UNTIL 5 DO IOUT[I]);
2700       WRITE(OUT,<I1>,N);
2800       WRITE(OUT,<I3>,M);
2900       WRITE(OUT,<I3>,P);
3000       WRITE(OUT,<I3>,II);
3100       WRITE(OUT,<I3>,III);
3200       WRITE(OUT,<F7.3>,V);
3300       WRITE(OUT,<F10.3>,TMAX);
3400       WRITE(OUT,<I6>,DCINT);
3500       WRITE(OUT,<F10.3>,DELTAT);
3600       WRITE(OUT,<6(I1,","),I1>,FOR I:=1 STEP 1 UNTIL 7 DO IOPT[I]);
3700       IF IOPT[1]=1 THEN WRITE(OUT,<F7.3>,D[1]) ELSE
3800       WRITE(OUT,<1(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO D[I]);
3900       IF IOPT[2]=1 THEN WRITE(OUT,<F10.3,",",F10.3>,AS[1],AE[1]) ELSE
4000       WRITE(OUT,<1(F7.3,",",F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N
4100            DO[AS[I],AE[I]]);
4200       IF IOPT[3]=1 THEN WRITE(OUT,<F7.3>,YCMIN[1]) ELSE
4300       WRITE(OUT,<1(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO YCMIN[I]);
4400       IF IOPT[4]=1 THEN WRITE(OUT,<F7.3>,YCMAX[1]) ELSE
4500       WRITE(OUT,<1(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO YCMAX[I]);
4600       IF IOPT[5]=1 THEN WRITE(OUT,<F7.3>,YEMIN[1]) ELSE
4700       WRITE(OUT,<1(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO YEMIN[I]);
4800       IF IOPT[6]=1 THEN WRITE(OUT,<F7.3>,YEMAX[1]) ELSE
4900       WRITE(OUT,<1(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO YEMAX[I]);
5000       WRITE(OUT,<I2>,INSR);
5100       IF INSR NEQ 0 THEN
5200       FOR I:=1 STEP 1 UNTIL INSR DO
5300       WRITE(OUT,<4(I1,","),F10.3>,R1[I],R2[I],P1[I],P2[I],SR[I]);
5400       IF IOPT[7]=1 THEN WRITE(OUT,<F11.5>,S[1,1]) ELSE
5500       FOR I:=1 STEP 1 UNTIL N DO
5600       WRITE(OUT,<1(F11.5,X1)>,FOR L:=1 STEP 1 UNTIL N DO S[I,L]);
5700       WRITE(OUT,<1(I1,X1)>,FOR I:=1 STEP 1 UNTIL N DO ICIN[I]);
5800       FOR I:=1 STEP 1 UNTIL N DO
5900         BEGIN
```

```
6000          IF ICIN[I]=0 THEN WRITE(OUT,<P11.5>,CO[I]);
6100          IF ICIN[I]=1 THEN
6200          WRITE(OUT,<I1,",",P10.3,",",P11.5>,IPORM[I],COTIME[I],CO[I]);
6300          IF ICIN[I]=2 THEN
6400          WRITE(OUT,<I1,",",I3,",",I3>,IPORM[I],IENPOI[I],ISTPOI[I]);
6500          IF ICIN[I]=2 AND IPORM[I]=0 THEN
6600          WRITE(OUT,<P11.5>,C[I,ISTPOI[I]]);
6700          IF ICIN[I]=2 AND IPORM[I]=1 THEN
6800          WRITE(OUT,<10(P10.5)>,FOR L:=IENPOI[I] STEP 1 UNTIL ISTPOI[I]
6900              DO C[I,L]);
7000        END;
7100    END PRINT;
7200
7300  PROCEDURE PRINTSCREEN;
7400    BEGIN
7500      WRITE(SCREEN,<A*>,LENGTH(TITLE),TITLE);
7600      WRITE(SCREEN,<"PLOTNAMEC=",A6,"  PLOTNAMEE=",A6>,PLNAC,PLNAE);
7700      WRITE(SCREEN,<"IOUT: ",5(I1,",")>,FOR I:=1 STEP 1 UNTIL 5 DO
7800           IOUT[I]);
7900      WRITE(SCREEN,<"N=",I1,"  POINTS=",I3,"  LENGTH=",I3>,N,M,P);
8000      WRITE(SCREEN,<"TIMESTEPC= ",I3,"  TIMESTEPE= ",I3>,II,III);
8100      WRITE(SCREEN,<"V=",P7.3,"  TMAX=",P10.3,"  DCINT=",I7," DELTAT=",
8200           P10.3>,V,TMAX,DCINT,DELTAT);
8300      WRITE(SCREEN,<"IOPT: ",7(I1,",")>,FOR I:=1 STEP 1 UNTIL 7 DO
8400           IOPT[I]);
8500      IF IOPT[1]=1 THEN WRITE(SCREEN,<"D=",F7.3>,D[1]) ELSE
8600      WRITE(SCREEN,<"D= ",5(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO D[I]);
8700      IF IOPT[2]=1 THEN
8800      WRITE(SCREEN,<"AS,AE= ",2P10.3,X1>,AS[1],AE[1]) ELSE
8900      WRITE(SCREEN,<"AS,AE= ",5(F7.3,X1,F7.3,X1)>,FOR I:=1 STEP 1 UNTIL
9000           N DO[AS[I],AE[I]]);
9100      IF IOPT[3]=1 THEN WRITE(SCREEN,<"YCMIN= ",F7.3>,YCMIN[1]) ELSE
9200      WRITE(SCREEN,<"YCMIN= ",5(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO
9300           YCMIN[I]);
9400      IF IOPT[4]=1 THEN WRITE(SCREEN,<"YCMAX= ",F7.3>,YCMAX[1]) ELSE
9500      WRITE(SCREEN,<"YCMAX= ",5(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO
9600           YCMAX[I]);
9700      IF IOPT[5]=1 THEN WRITE(SCREEN,<"YEMIN= ",F7.3>,YEMIN[1]) ELSE
9800      WRITE(SCREEN,<"YEMIN= ",5(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO
9900           YEMIN[I]);
10000      IF IOPT[6]=1 THEN WRITE(SCREEN,<"YEMAX= ",F7.3>,YEMAX[1]) ELSE
10100      WRITE(SCREEN,<"YEMAX= ",5(F7.3,X1)>,FOR I:=1 STEP 1 UNTIL N DO
10200           YEMAX[I]);
10300      WRITE(SCREEN,<"NUMBER OF SO-REACTIONS= ",I2>,INSR);
10400      IF INSR NEQ 0 THEN
10500      FOR I:=1 STEP 1 UNTIL INSR DO
10600      WRITE(SCREEN,<"R",I1,4(X1,I1),P10.3>,I,R1[I],R2[I],P1[I],P2[I],
10700           SR[I]);
10800      IF IOPT[7]=1 THEN WRITE(SCREEN,<"S= ",P11.5>,S[1,1]) ELSE
10900      FOR I:=1 STEP 1 UNTIL N DO
11000      WRITE(SCREEN,<"S= ",5(P11.5,X1)>,FOR L:=1 STEP 1 UNTIL N DO
11100           S[I,L]);
11200      WRITE(SCREEN,<"ICIN= ",5(I1,X1)>,FOR I:=1 STEP 1 UNTIL N DO
11300           ICIN[I]);
11400      FOR I:=1 STEP 1 UNTIL N DO
11500        BEGIN
11600          IF ICIN[I]=0 THEN WRITE(SCREEN,<"C= ",P11.5>,CO[I]);
11700          IF ICIN[I]=1 THEN
11800          WRITE(SCREEN,<"IPORM= ",I1,"  COTIME= ",P10.3,"  C= ",P11.5>,
```

```
11900              IFORM[I],COTIME[I],CO[I]);
12000            IF ICIN[I]=2 THEN
12100            WRITE(SCREEN,<"IFORM= ",I1,"  ENDPOINT= ",I3,"  STARTPOINT= ",
12200                I3>,IFORM[I],IENPOI[I],ISTPOI[I]);
12300            IF ICIN[I]=2 AND IFORM[I]=0 THEN
12400            WRITE(SCREEN,<"C= ",F11.5>,C[I,ISTPOI[I]]);
12500            IF ICIN[I]=2 AND IFORM[I]=1 THEN
12600            WRITE(SCREEN,<"C= ",10(F10.5)>,FOR L:=IENPOI[I] STEP 1 UNTIL
12700                ISTPOI[I] DO C[I,L]);
12800          END;
12900      END PRINTSCREEN;
13000
13100    PROCEDURE READFILE;
13200      BEGIN
13300        READ(INP,<A70>,TITLE);
13400        READ(INP,<A6>,PLNAC);
13500        READ(INP,<A6>,PLNAE);
13600        READ(INP,/,IOUT[1],IOUT[2],IOUT[3],IOUT[4],IOUT[5]);
13700        READ(INP,/,N);
13800        READ(INP,/,M);
13900        READ(INP,/,P);
14000        READ(INP,/,II);
14100        READ(INP,/,III);
14200        READ(INP,/,V);
14300        READ(INP,/,TMAX);
14400        READ(INP,/,DCINT);
14500        READ(INP,/,DELTAT);
14600        READ(INP,/,IOPT[1],IOPT[2],IOPT[3],IOPT[4],IOPT[5],IOPT[6],
14700            IOPT[7]);
14800        I:=1;
14900        IF IOPT[1]=1 THEN READ(INP,/,D[1]);
15000        IF IOPT[1]=0 THEN READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO D[I]);
15100        IF IOPT[2]=1 THEN READ(INP,/,AS[1],AE[1]);
15200        IF IOPT[2]=0 THEN
15300        READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO[AS[I],AE[I]]);
15400        IF IOPT[3]=1 THEN READ(INP,/,YCMIN[1]);
15500        IF IOPT[3]=0 THEN
15600        READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO YCMIN[I]);
15700        IF IOPT[4]=1 THEN READ(INP,/,YCMAX[1]);
15800        IF IOPT[4]=0 THEN
15900        READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO YCMAX[I]);
16000        IF IOPT[5]=1 THEN READ(INP,/,YEMIN[1]);
16100        IF IOPT[5]=0 THEN
16200        READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO YEMIN[I]);
16300        IF IOPT[6]=1 THEN READ(INP,/,YEMAX[1]);
16400        IF IOPT[6]=0 THEN
16500        READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO YEMAX[I]);
16600        READ(INP,/,INSR);
16700        IF INSR NEQ 0 THEN
16800        FOR I:=1 STEP 1 UNTIL INSR DO
16900        READ(INP,/,R1[I],R2[I],P1[I],P2[I],SR[I]);
17000        IF IOPT[7]=1 THEN READ(INP,/,S[1,1]);
17100        IF IOPT[7]=0 THEN
17200        FOR I:=1 STEP 1 UNTIL N DO
17300        READ(INP,/,FOR L:=1 STEP 1 UNTIL N DO S[I,L]);
17400        READ(INP,/,FOR I:=1 STEP 1 UNTIL N DO ICIN[I]);
17500        FOR I:=1 STEP 1 UNTIL N DO
17600          BEGIN
17700            IF ICIN[I]=0 THEN READ(INP,/,CO[I]);
```

```
17800           IF ICIN[I]=1 THEN READ(INP,/,IFORM[I],COTIME[I],CO[I]);
17900           IF ICIN[I]=2 THEN READ(INP,/,IFORM[I],IENPOI[I],ISTPOI[I]);
18000           IF ICIN[I]=2 AND IFORM[I]=0 THEN READ(INP,/,C[I,ISTPOI[I]]);
18100           IF ICIN[I]=2 AND IFORM[I]=1 THEN
18200           READ(INP,/,FOR L:=IENPOI[I] STEP 1 UNTIL ISTPOI[I] DO C[I,L]);
18300         END;
18400     END READFILE;
18500 $BEGINSEGMENT
18600
18700   BOOLEAN PROCEDURE PARSEINPUT(INARRAY,OUTFILE,ERRORLIMIT);
18800 %                  ############################
18900   VALUE ERRORLIMIT;
19000   INTEGER ERRORLIMIT;
19100   ARRAY INARRAY[*];
19200   FILE OUTFILE;
19300     BEGIN
19400       STRING NAMEVALUE,RESERVEDWORDVALUE,LITERALVALUE;
19500       REAL NUMBERVALUE;
19600       BOOLEAN ENDOFFILEVALUE,PARSEDONE,SYNTAXERROR,
19700       INTEGER STRINGLENGTH,CURRENTSTATE,COLUMNLEFT,INDEX,ARRAYSIZE,
19800             STARTCOLUMN,ENDCOLUMN;
19900       POINTER TOKENP,ENDP,STRINGP;
20000       TRUTHSET NUMBERS("0123456789.+-@"),DIGIT("0123456789"),
20100             LETTERS(ALPHA AND NOT DIGIT);
20200       DEFINE RESERVEDWORDF=47:16#,OVERFLOWF=31:16#,TYPEVALUEF=15:16#;
20300       DEFINE NEXTSTATEF=47:12#,INPUTVALUEF=35:12#,STATEF=23:12#,
20400            CASENUMF=11:12#;
20500       DEFINE TOKENV=0#,SYNTAXV=1#,SEMANTICV=2#;
20600       DEFINE NAMEV=0#,NUMBERV=1#,LITV=2#,EOFV=3#;
20700  $INCLUDE "SYMBOL/TABLES"
20800 %############################
20900
21000       PROCEDURE SEMANTICS(WHICH);
21100       VALUE WHICH;
21200       INTEGER WHICH;
21300       FORWARD;
21400
21500       PROCEDURE ERROR(ERRORMESSAGE);
21600       VALUE ERRORMESSAGE;
21700       STRING ERRORMESSAGE;
21800       FORWARD;
21900       DEFINE HASHIT=INDEX:=(REAL(TOKENP,MIN(STRINGLENGTH,4))+
22000             STRINGLENGTH) MOD HASHMODV#;
22100
22200       INTEGER PROCEDURE LOOKUP;
22300 %                  #######
22400         BEGIN
22500           BOOLEAN MATCHFOUND;
22600           HASHIT;
22700           DO
22800             BEGIN
22900               STRINGP:=POINTER(RESERVEDWORDS)+
23000                       HASHTABLE[INDEX].[RESERVEDWORDF];
23100               IF STRINGLENGTH=INTEGER(STRINGP:STRINGP,2) THEN
23200               IF TOKENP=STRINGP FOR STRINGLENGTH THEN
23300                 BEGIN
23400                   MATCHFOUND:=TRUE;
23500                   LOOKUP:=HASHTABLE[INDEX].[TYPEVALUEF];
23600                 END;
```

```
23700             END UNTIL MATCHFOUND OR
23800                 INDEX:=HASHTABLE[INDEX].[OVERFLOWF]=4"FFFF";
23900           IF NOT MATCHFOUND THEN
24000           IF TOKENP IN LETTERS THEN LOOKUP:=NAMEV ELSE
24100             BEGIN
24200               LOOKUP:=-1;
24300               ERROR("** UNRECOGNIZED SYNTAX **");
24400             END;
24500         END LOOKUP;
24600
24700       INTEGER PROCEDURE GETTOKEN;
24800         BEGIN
24900           DEFINE EOFTOKEN=48"00"#;
25000           SCAN TOKENP:ENDP FOR COLUMNLEFT:COLUMNLEFT WHILE=" ";
25100           STARTCOLUMN:=ARRAYSIZE-COLUMNLEFT;
25200           IF(IF COLUMNLEFT=0 THEN TRUE ELSE TOKENP=EOFTOKEN)THEN
25300             BEGIN
25400               GETTOKEN:=EOFV;
25500               ENDOFFILEVALUE:=TRUE;
25600             END
25700           ELSE
25800           IF(IF TOKENP IN DIGIT FOR 1 THEN TRUE ELSE
25900           TOKENP IN NUMBERS FOR 2) THEN
26000             BEGIN
26100               SCAN ENDP:TOKENP FOR COLUMNLEFT:COLUMNLEFT WHILE IN
26200                   NUMBERS;
26300               ENDCOLUMN:=ARRAYSIZE-COLUMNLEFT;
26400               IF STRINGLENGTH:=ENDCOLUMN-STARTCOLUMN>13 THEN
26500                 BEGIN
26600                   GETTOKEN:=-1;
26700                   ERROR("** ILLEGAL NUMBER **");
26800                 END
26900               ELSE
27000                 BEGIN
27100                   GETTOKEN:=NUMBERV;
27200                   NUMBERVALUE:=DECIMAL(STRING(TOKENP,STRINGLENGTH));
27300                 END;
27400             END
27500           ELSE
27600           IF TOKENP IN LETTERS THEN
27700             BEGIN
27800               SCAN ENDP:TOKENP FOR COLUMNLEFT:COLUMNLEFT WHILE IN ALPHA;
27900               ENDCOLUMN:=ARRAYSIZE-COLUMNLEFT;
28000               STRINGLENGTH:=ENDCOLUMN-STARTCOLUMN;
28100               IF(GETTOKEN:=LOOKUP)=NAMEV THEN
28200               NAMEVALUE:=STRING(TOKENP,STRINGLENGTH) ELSE
28300               RESERVEDWORDVALUE:=STRING(TOKENP,STRINGLENGTH);
28400             END
28500           ELSE
28600           IF TOKENP="""" THEN
28700             BEGIN
28800               IF COLUMNLEFT>0 THEN
28900                 BEGIN
29000                   STARTCOLUMN:=*+1;
29100                   TOKENP:=TOKENP+1;
29200                   COLUMNLEFT:=*-1;
29300                 END;
29400               SCAN ENDP:TOKENP FOR COLUMNLEFT:COLUMNLEFT UNTIL="""";
29500               ENDCOLUMN:=ARRAYSIZE-COLUMNLEFT;
```

```
29600              IF COLUMNLEFT=0 OR STRINGLENGTH:=ENDCOLUMN-STARTCOLUMN=0
29700                THEN
29800                BEGIN
29900                  GETTOKEN:=-1;
30000                  ERROR("** MISSING END QUOTE **");
30100                END
30200              ELSE
30300                BEGIN
30400                  GETTOKEN:=LITV;
30500                  LITERALVALUE:=STRING(TOKENP,STRINGLENGTH);
30600                  IF COLUMNLEFT>0 THEN
30700                    BEGIN
30800                      ENDP:=ENDP+1;
30900                      COLUMNLEFT:=*-1;
31000                    END;
31100                END;
31200            END
31300          ELSE
31400            BEGIN
31500              STRINGLENGTH:=1;
31600              IF COLUMNLEFT>0 THEN
31700                BEGIN
31800                  COLUMNLEFT:=*-1;
31900                  ENDP:=TOKENP+1;
32000                END;
32100              GETTOKEN:=LOOKUP;
32200              RESERVEDWORDVALUE:=STRING(TOKENP,STRINGLENGTH);
32300            END SPECIAL CHARACTER;
32400        END GETTOKEN;
32500
32600      PROCEDURE PARSE;
32700        BEGIN
32800          INTEGER TOKEN,RULE;
32900          IF TOKEN:=GETTOKEN GEQ 0 THEN
33000            BEGIN
33100              IF
33200 RULE:=ARRAYSEARCH(0&TOKEN[INPUTVALUEP]&CURRENTSTATE[STATEP],
33300                  0&4"FFF"[INPUTVALUEP]&4"FFF"[STATEP],GRAMMAR)<0 THEN
33400                IF TOKEN=EOFV THEN
33500                  BEGIN
33600                    STRINGLENGTH:=1;
33700                    ERROR("** MORE INPUT REQUIRED **");
33800                  END
33900                ELSE ERROR("** UNEXPECTED INPUT IN THIS CONTEXT **") ELSE
34000                  BEGIN
34100                    CURRENTSTATE:=GRAMMAR[RULE].[NEXTSTATEP];
34200                    IF RULE:=GRAMMAR[RULE].[CASENUMF] NEQ 4"FFF" THEN
34300                    SEMANTICS(RULE);
34400                  END;
34500              END;
34600        END PARSE;
34700
34800      PROCEDURE SEMANTICS(WHICH);
34900 %        ##################
35000      VALUE WHICH;
35100      INTEGER WHICH;
35200        BEGIN
35300          CASE WHICH OF
35400            BEGIN
```

```
35500 1:            INPUTFINISHED:=PARSEDONE:=TRUE;
35600 2:            REMOTEINPUT:=TRUE;
35700 3:            REMOTEINPUT:=FALSE;
35800               INPUTTITLE:=LITERALVALUE;
35900 4:            OUTPUTTITLE:=LITERALVALUE;
36000 10:           TITLE:=LITERALVALUE;
36100 11:           PLNAC:=NAMEVALUE;
36200 12:           PLNAE:=NAMEVALUE;
36300 13:           INPUTPRINT:=RESERVEDWORDVALUE="NO";
36400 14:           IOUT[2]:=NUMBERVALUE;
36500 15:           NEGCON:=RESERVEDWORDVALUE="NO";
36600               IF NEGCON THEN IOUT[3]:=1 ELSE IOUT[3]:=0;
36700 16:           INTEGRATION:=RESERVEDWORDVALUE="NO";
36800               IF INTEGRATION THEN IOUT[4]:=0 ELSE IOUT[4]:=1;
36900 17:           HARDPLOT:=RESERVEDWORDVALUE="NO";
37000               IF HARDPLOT THEN IOUT[5]:=0 ELSE IOUT[5]:=1;
37100 18:           N:=NUMBERVALUE;
37200 19:           M:=NUMBERVALUE;
37300 20:           P:=NUMBERVALUE;
37400 21:           II:=NUMBERVALUE;
37500 22:           III:=NUMBERVALUE;
37600 23:           V:=NUMBERVALUE;
37700 24:           TMAX:=NUMBERVALUE;
37800 25:           DELTAT:=NUMBERVALUE;
37900 26:           IOPT[1]:=0;
38000               FOR I:=1 STEP 1 UNTIL N DO
38100                 BEGIN
38200                   WRITE(SCREEN,<"DISPERSION COEFFICIENT OF COMPONENT ",
38300                         I1," ?">,I);
38400                   READ(KEYBOARD,/,D[I]);
38500                 END;
38600 27:           IOPT[2]:=0;
38700               FOR I:=1 STEP 1 UNTIL N DO
38800                 BEGIN
38900                   WRITE(SCREEN,<"AS AND AE OF COMPONENT ",I1," ?">,I);
39000                   READ(KEYBOARD,/,AS[I],AE[I]);
39100                 END;
39200 28:           IOPT[3]:=0;
39300               FOR I:=1 STEP 1 UNTIL N DO
39400                 BEGIN
39500                   WRITE(SCREEN,<"YCMIN OF COMPONENT ",I1," ?">,I);
39600                   READ(KEYBOARD,/,YCMIN[I]);
39700                 END;
39800 29:           IOPT[4]:=0;
39900               FOR I:=1 STEP 1 UNTIL N DO
40000                 BEGIN
40100                   WRITE(SCREEN,<"YCMAX OF COMPONENT ",I1," ?">,I);
40200                   READ(KEYBOARD,/,YCMAX[I]);
40300                 END;
40400 30:           IOPT[5]:=0;
40500               FOR I:=1 STEP 1 UNTIL N DO
40600                 BEGIN
40700                   WRITE(SCREEN,<"YEMIN OF COMPONENT ",I1," ?">,I);
40800                   READ(KEYBOARD,/,YEMIN[I]);
40900                 END;
41000 31:           IOPT[6]:=0;
41100               FOR I:=1 STEP 1 UNTIL N DO
41200                 BEGIN
41300                   WRITE(SCREEN,<"YEMAX OF COMPONENT ",I1," ?">,I);
```

```
41400                   READ(KEYBOARD,/,YEMAX[I]);
41500                 END;
41600 32:           IOPT[7]:=0;
41700               FOR I:=1 STEP 1 UNTIL N DO
41800                 BEGIN
41900                   FOR L:=1 STEP 1 UNTIL N DO
42000                   WRITE(SCREEN,<"S[",I1,",",I1,"]  ?">,I,L);
42100                   READ(KEYBOARD,/,FOR L:=1 STEP 1 UNTIL N DO S[I,L]);
42200                 END;
42300 33:           D[1]:=NUMBERVALUE;
42400 34:           AS[1]:=NUMBERVALUE;
42500 35:           AE[1]:=NUMBERVALUE;
42600 36:           YCMIN[1]:=NUMBERVALUE;
42700 37:           YCMAX[1]:=NUMBERVALUE;
42800 38:           YEMIN[1]:=NUMBERVALUE;
42900 39:           YEMAX[1]:=NUMBERVALUE;
43000 40:           INSR:=NUMBERVALUE;
43100               IF INSR NEQ 0 THEN
43200               FOR I:=1 STEP 1 UNTIL INSR DO
43300                 BEGIN
43400                   WRITE(SCREEN,<"NUMBER OF REACTANT ONE ?">);
43500                   READ(KEYBOARD,/,R1[I]);
43600                   WRITE(SCREEN,<"NUMBER OF REACTANT TWO ?">);
43700                   READ(KEYBOARD,/,R2[I]);
43800                   WRITE(SCREEN,<"NUMBER OF PRODUCT ONE ?">);
43900                   READ(KEYBOARD,/,P1[I]);
44000                   WRITE(SCREEN,<"NUMBER OF PRODUCT TWO ?">);
44100                   READ(KEYBOARD,/,P2[I]);
44200                   WRITE(SCREEN,<"RATE CONSTANT FOR REACTION ",I2,"  ?">,
44300                     I);
44400                   READ(KEYBOARD,/,SR[I]);
44500                 END;
44600 41:           S[1,1]:=NUMBERVALUE;
44700 42:
44800               WRITE(SCREEN,
44900                 <"0:CONTINIOUS-INPUT ,1:TIME-INPUT ,2:POINT INPUT">);
45000               FOR I:=1 STEP 1 UNTIL N DO
45100                 BEGIN
45200                   WRITE(SCREEN,<"INPUT TYPE OF COMPONENT ",I1,
45300                     "   0,1,OR 2 ?">,I);
45400                   READ(KEYBOARD,/,ICIN[I]);
45500                   IF ICIN[I]=0 THEN
45600                     BEGIN
45700                       WRITE(SCREEN,<"CONCENTRATION ?">);
45800                       READ(KEYBOARD,/,CO[I]);
45900                     END;
46000                   IF ICIN[I]=1 THEN
46100                     BEGIN
46200                       WRITE(SCREEN,<"TIME ? AND CONCENTRATION ?">);
46300                       READ(KEYBOARD,/,COTIME[I],CO[I]);
46400                       IFORM[I]:=1;
46500                     END;
46600                   IF ICIN[I]=2 THEN
46700                     BEGIN
46800                       WRITE(SCREEN,
46900                         <"FORM (0 OR 1) ? ENDPOINT ? STARTPOINT ?">);
47000                       READ(KEYBOARD,/,IFORM[I],IENPOI[I],ISTPOI[I]);
47100                       IF IFORM[I]=0 THEN
47200                       WRITE(SCREEN,<"CONCENTRATION ?">);
```

```
47300                     IF IFORM[I]=0 THEN
47400                     READ(KEYBOARD,/,C[I,ISTPOI[I]]);
47500                     IF IFORM[I]=1 THEN
47600                     FOR L:=IENPOI[I] STEP 1 UNTIL ISTPOI[I] DO
47700                       BEGIN
47800                         WRITE(SCREEN,<"CONCENTRATION AT ",I3,"  ?">,
47900                              L);
48000                         READ(KEYBOARD,/,C[I,L]);
48100                       END;
48200                   END;
48300               END;
48400 46:           PRINTSCREEN;
48500 47:           IF NOT INPUTFINISHED THEN
48600               IF NOT REMOTEINPUT THEN
48700                 BEGIN
48800                   CLOSE(INP);
48900                   REPLACE PT:=POINTER(TITLEAR) BY INPUTTITLE,".";
49000                   INP(FILETYPE=7,TITLE=PT);
49100                   READFILE;
49200                 END;
49300 48:           REPLACE PT:=POINTER(TITLEAR) BY OUTPUTTITLE,".";
49400               OUT(NEWFILE=FALSE,TITLE=PT);
49500               IF OUT.RESIDENT THEN
49600                 BEGIN
49700                   WRITE(SCREEN,
49800                        <"RESIDENT FILE ! OVERWRITE ?  YES=1; NO=0;">);
49900                   READ(KEYBOARD,/,J);
50000                   IF J=1 THEN CLOSE(OUT,PURGE);
50100                 END
50200               ELSE J:=1;
50300               IF J=1 THEN
50400                 BEGIN
50500                   OUT(NEWFILE=TRUE);
50600                   PRINT(OUT);
50700                   LOCK(OUT,CRUNCH);
50800                 END;
50900             END CASE;
51000           IF WHICH GEQ 10 THEN PARSEDONE:=TRUE;
51100         END SEMANTICS;
51200
51300       PROCEDURE ERROR(ERRORMESSAGE);
51400 %         ##################
51500       VALUE ERRORMESSAGE;
51600       STRING ERRORMESSAGE;
51700         BEGIN
51800           ARRAY UNDERLINE[0:12];
51900           POINTER P,PSTART;
52000           INTEGER UNITSPERWORD;
52100           UNITSPERWORD:=IF OUTFILE.UNITS=VALUE(CHARACTERS) THEN 6 ELSE
52200           1;
52300           REPLACE P:=POINTER(UNDERLINE) BY "      " FOR 13 WORDS;
52400           IF OFFSET(TOKENP)+STRINGLENGTH>78 THEN
52500           PSTART:=TOKENP-MIN(50,OFFSET(TOKENP)) ELSE
52600           PSTART:=POINTER(INARRAY);
52700           WRITE(OUTFILE,(MIN(ARRAYSIZE-OFFSET(PSTART),78)+5)DIV 6*
52800                UNITSPERWORD,PSTART);
52900           REPLACE P+(OFFSET(TOKENP)-OFFSET(PSTART)) BY "#" FOR
53000                MIN(STRINGLENGTH,5);
53100           WRITE(OUTFILE,13*UNITSPERWORD,UNDERLINE);
```

```
53200           WRITE(OUTFILE,13*UNITSPERWORD,ERRORMESSAGE CAT REPEAT(" ",72-
53300                LENGTH(ERRORMESSAGE)));
53400           SYNTAXERROR:=TRUE;
53500           ENDOFFILEVALUE:=TRUE;
53600           IF(ERRORLIMIT:=*-1)=0 THEN PARSEDONE:=TRUE;
53700         END ERRORS;
53800 %
53900 %
54000 %
54100       ARRAYSIZE:=6*SIZE(INARRAY);
54200       COLUMNLEFT:=ARRAYSIZE;
54300       ENDP:=POINTER(INARRAY);
54400       DO PARSE UNTIL PARSEDONE;
54500       PARSEINPUT:=NOT SYNTAXERROR;
54600     END OF P A R S E I N P U T;
54700 $ENDSEGMENT
54800
54900   PROCEDURE READINPUT;
55000     BEGIN
55100       COMMENT***DEFAULTS***;
55200       FOR I:=1 STEP 1 UNTIL 7 DO IOPT[I]:=1;
55300       FOR I:=1 STEP 1 UNTIL 5 DO IOUT[I]:=IFORM[I]:=1;
55400       IOUT[2]:=2;
55500       DCINT:=100000;
55600       M:=401;
55700       N:=1;
55800       REMOTEJOB:=MYSELF.STATION<0;
55900       REMOTEINPUT:=REMOTEJOB;
56000       IF REMOTEINPUT THEN KEYBOARD.OPEN:=TRUE;
56100       INPUTFINISHED:=FALSE;
56200       PC:=POINTER(CARD);
56300       WHILE NOT INPUTFINISHED DO
56400         BEGIN
56500           FILEFINISHED:=FALSE;
56600           IF REMOTEINPUT THEN
56700             BEGIN
56800               WRITE(SCREEN[STOP],<">">);
56900               READ(KEYBOARD,72,PC);
57000             END
57100           ELSE
57200             BEGIN
57300               FILEFINISHED:=READ(INP,<A72>,PC);
57400               IF FILEFINISHED THEN
57500                 BEGIN
57600                   IF REMOTEJOB THEN REMOTEINPUT:=TRUE ELSE
57700                   INPUTFINISHED:=TRUE;
57800                 END;
57900             END;
58000           IF NOT INPUTFINISHED AND NOT FILEFINISHED THEN
58100           PARSEINPUT(CARD,SCREEN,1);
58200         END WHILE;
58300     END READINPUT;
58400   READINPUT;
58500 END.
#
```

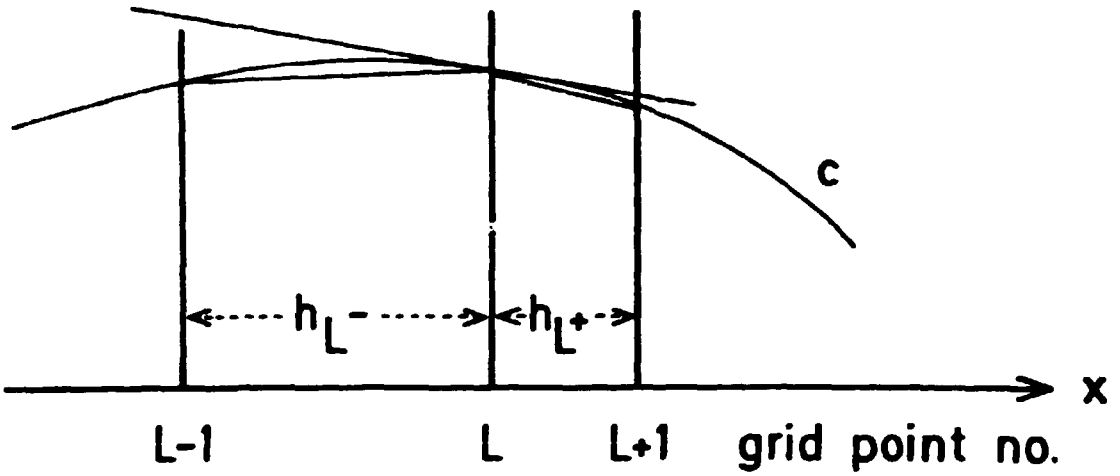

Fig. 3.1. Interpolation between non-equidistant grid points.

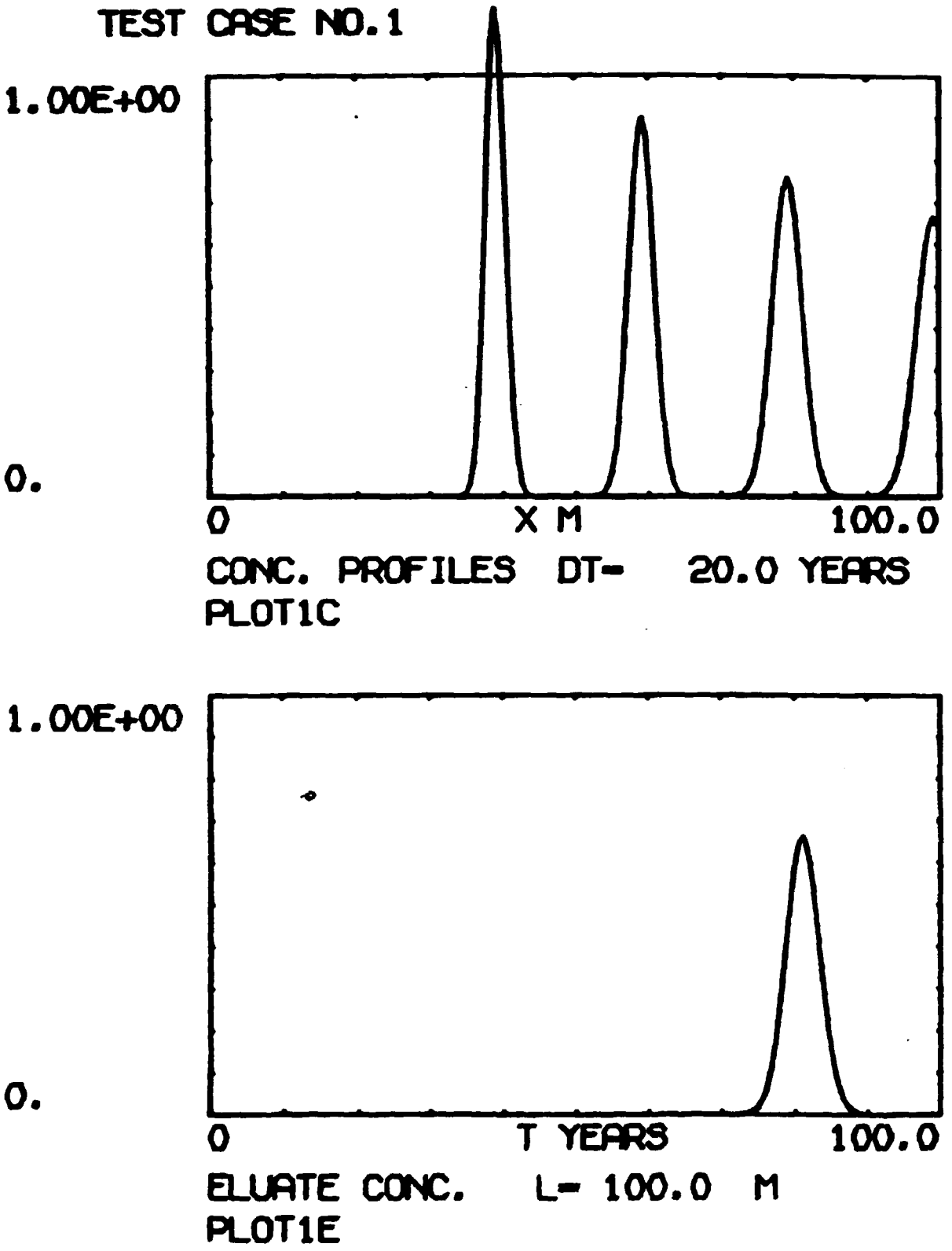

Fig. 6.1. Plotted output from test example 1

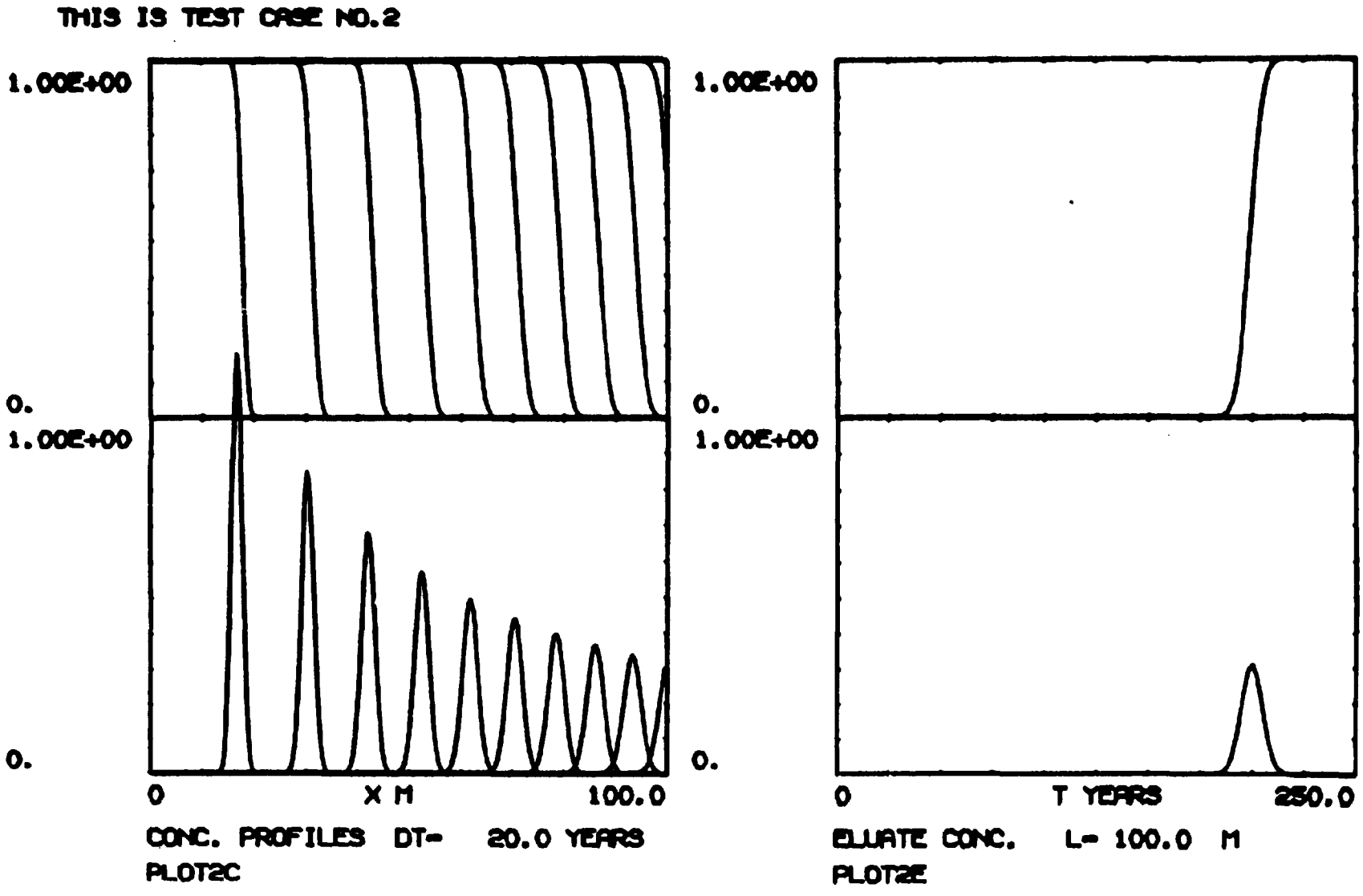

Fig. 6.2. Plotted output from test example 2

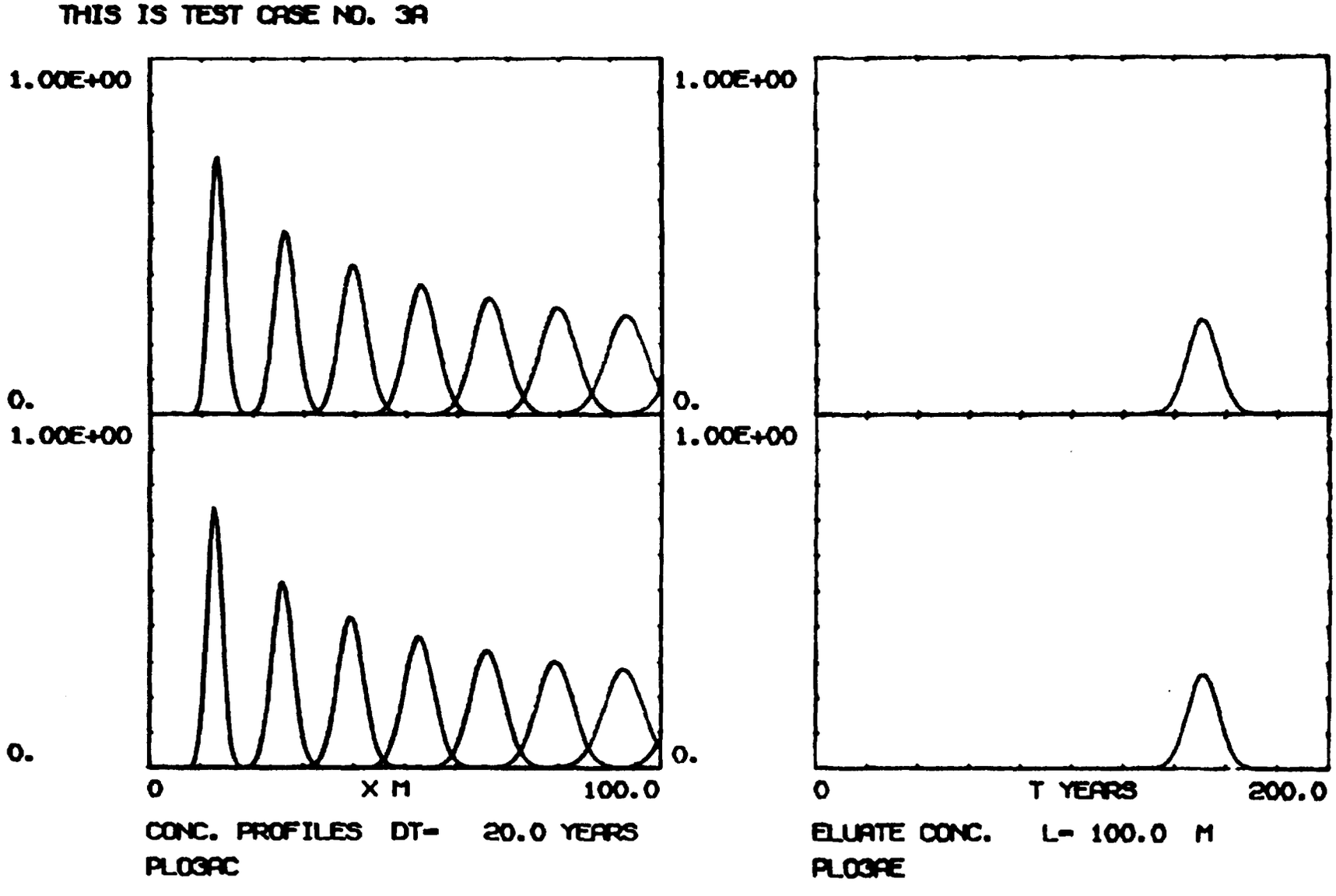

Fig. 6.3. Plotted output from test example 3A

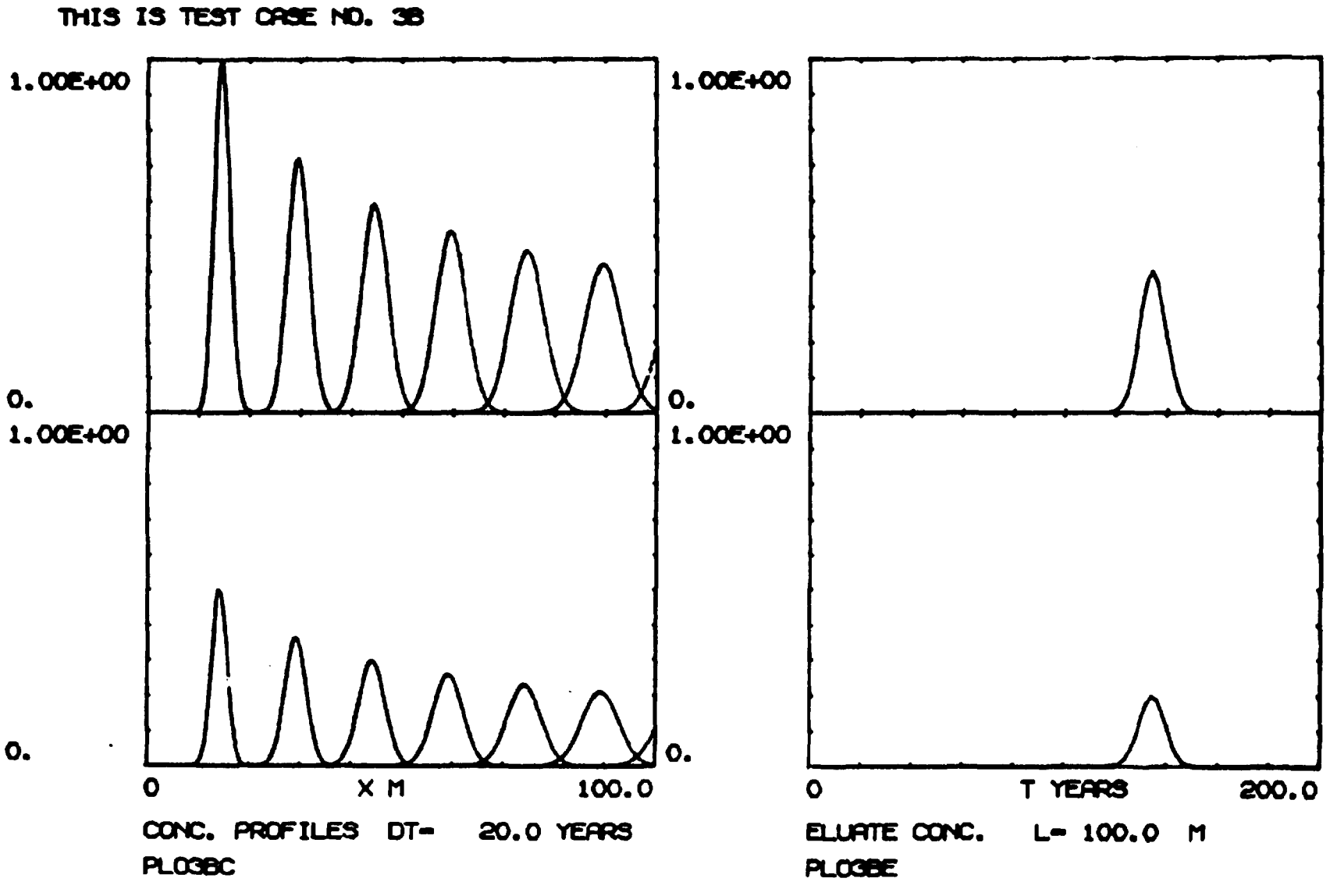

Fig. 6.4. Plotted output from test example 3B

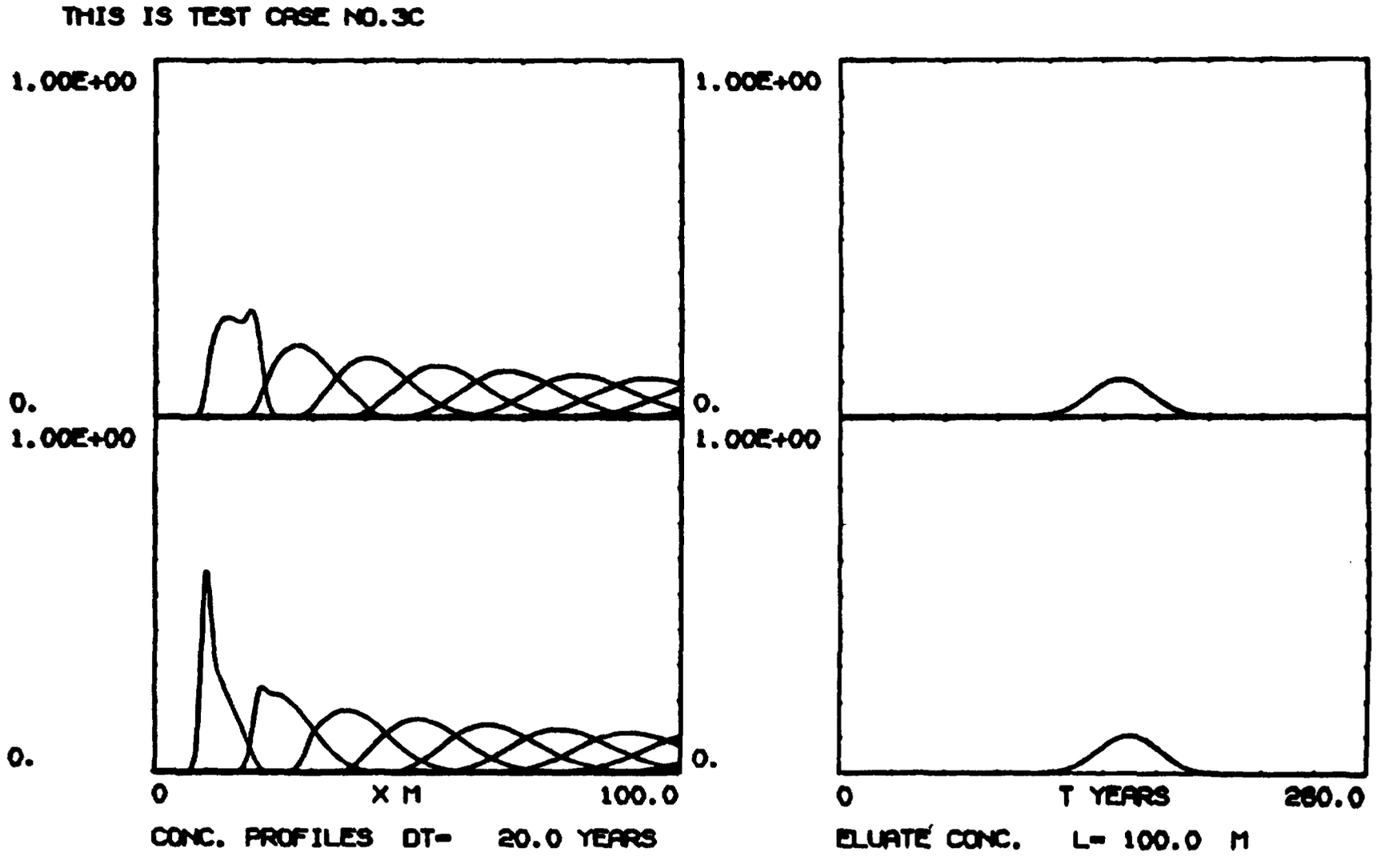

Fig. 6.5. Plotted output from test example 3C

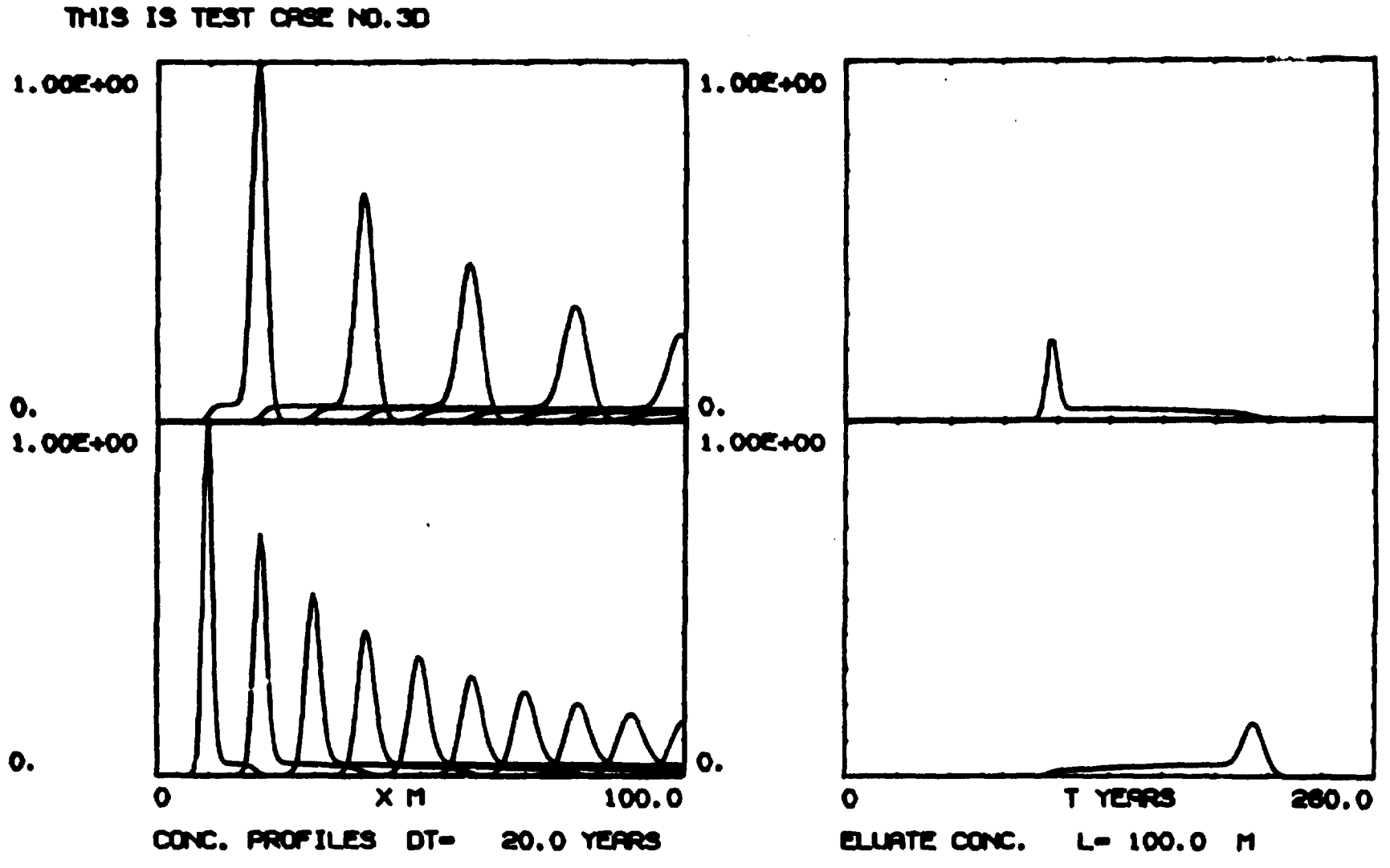

Fig. 6.6. Plotted output from test example 3D

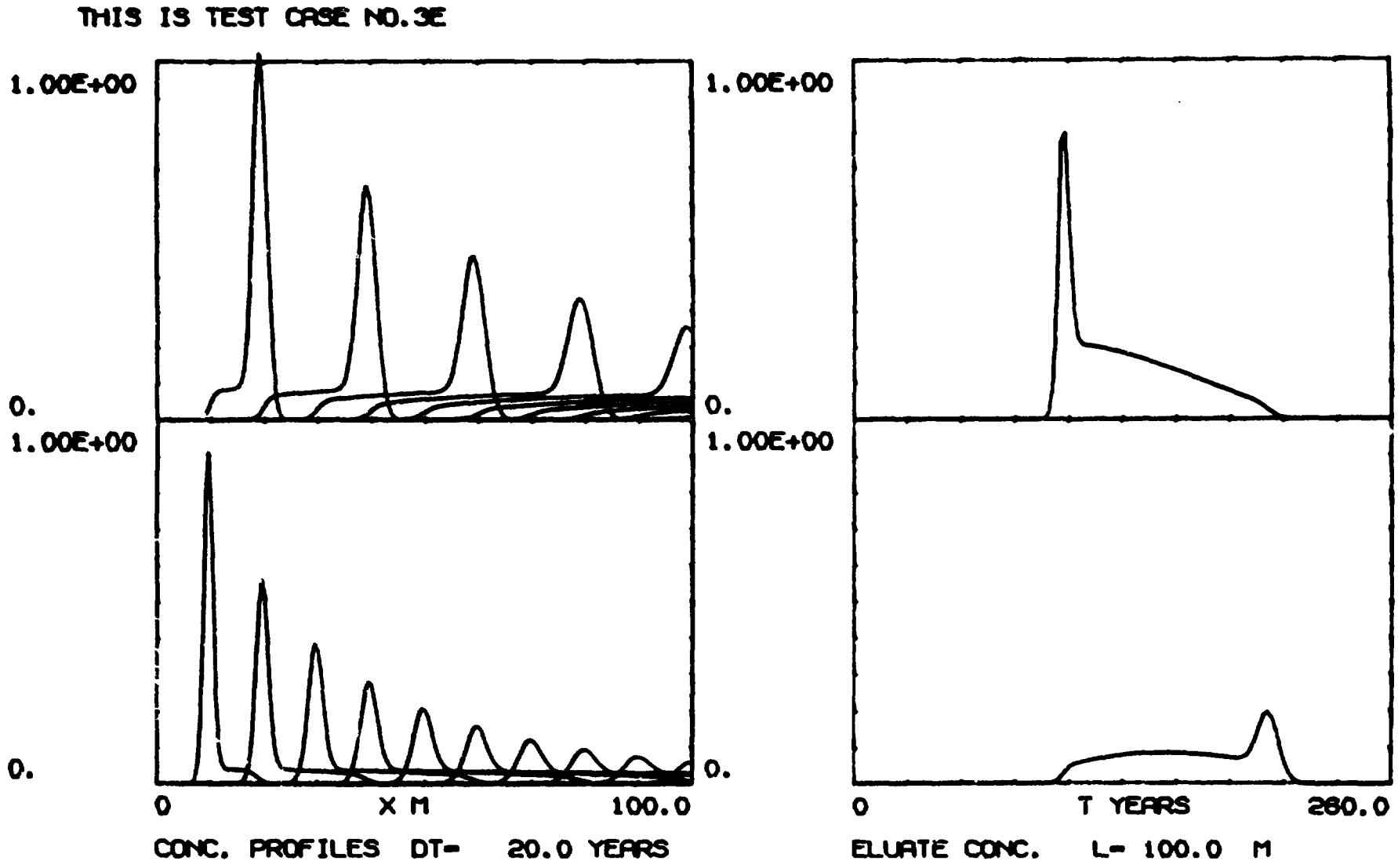

Fig. 6.7. Plotted output from test example 3a

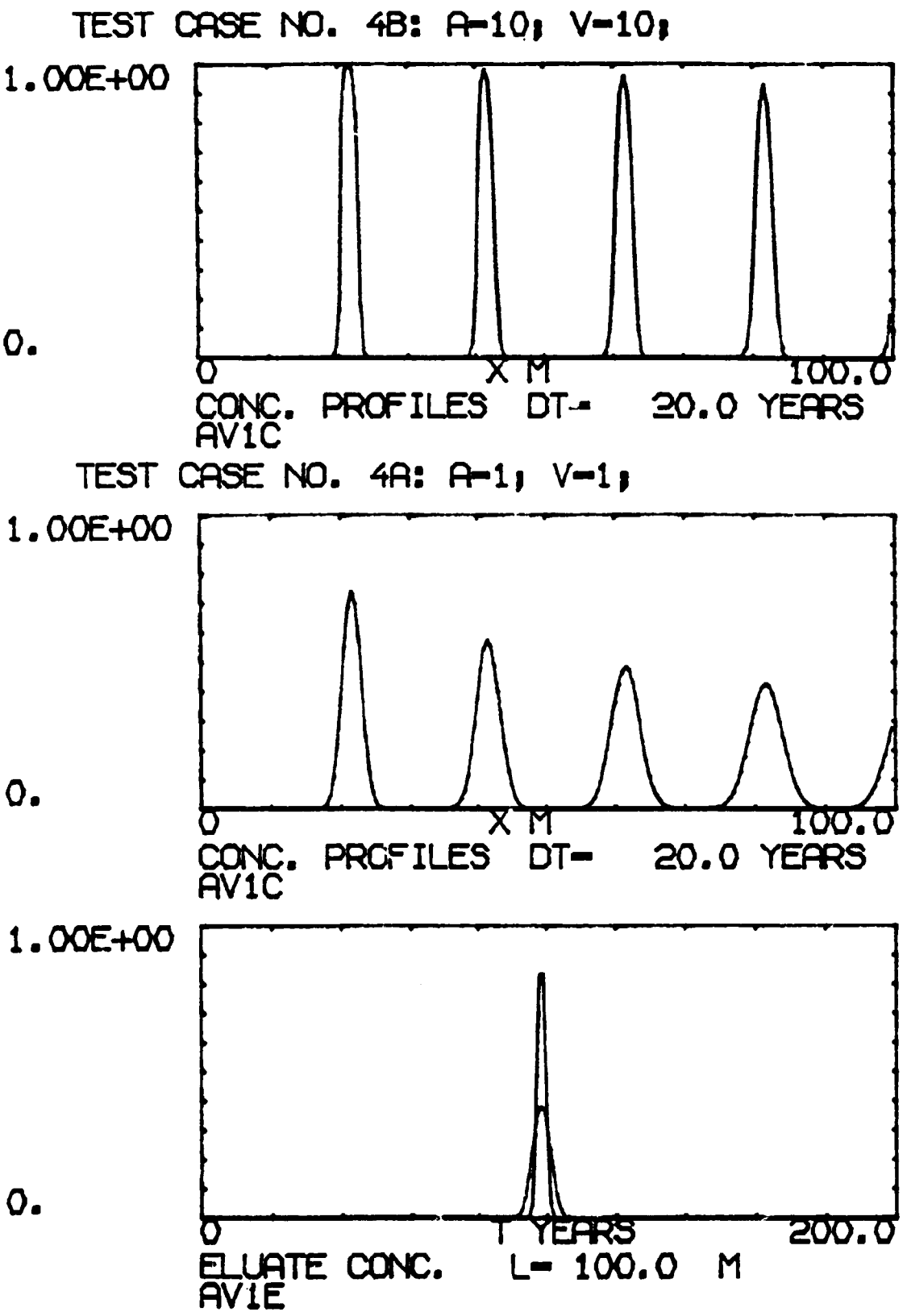

Fig. 6.8. Plotted output output from test example 4A and 4B

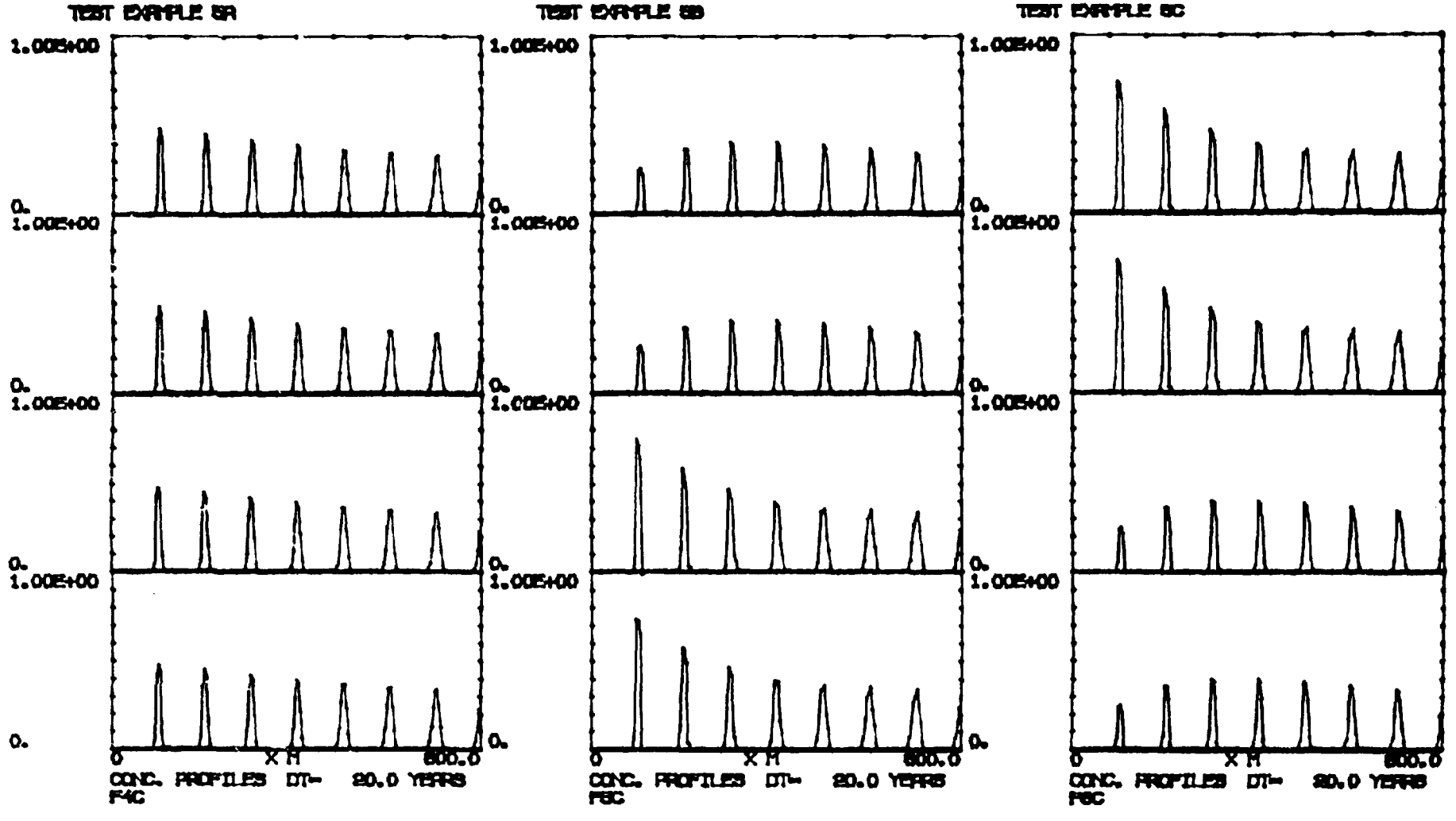

Fig. 6.9. Plotted output from test example 5A, 5B, and 5C

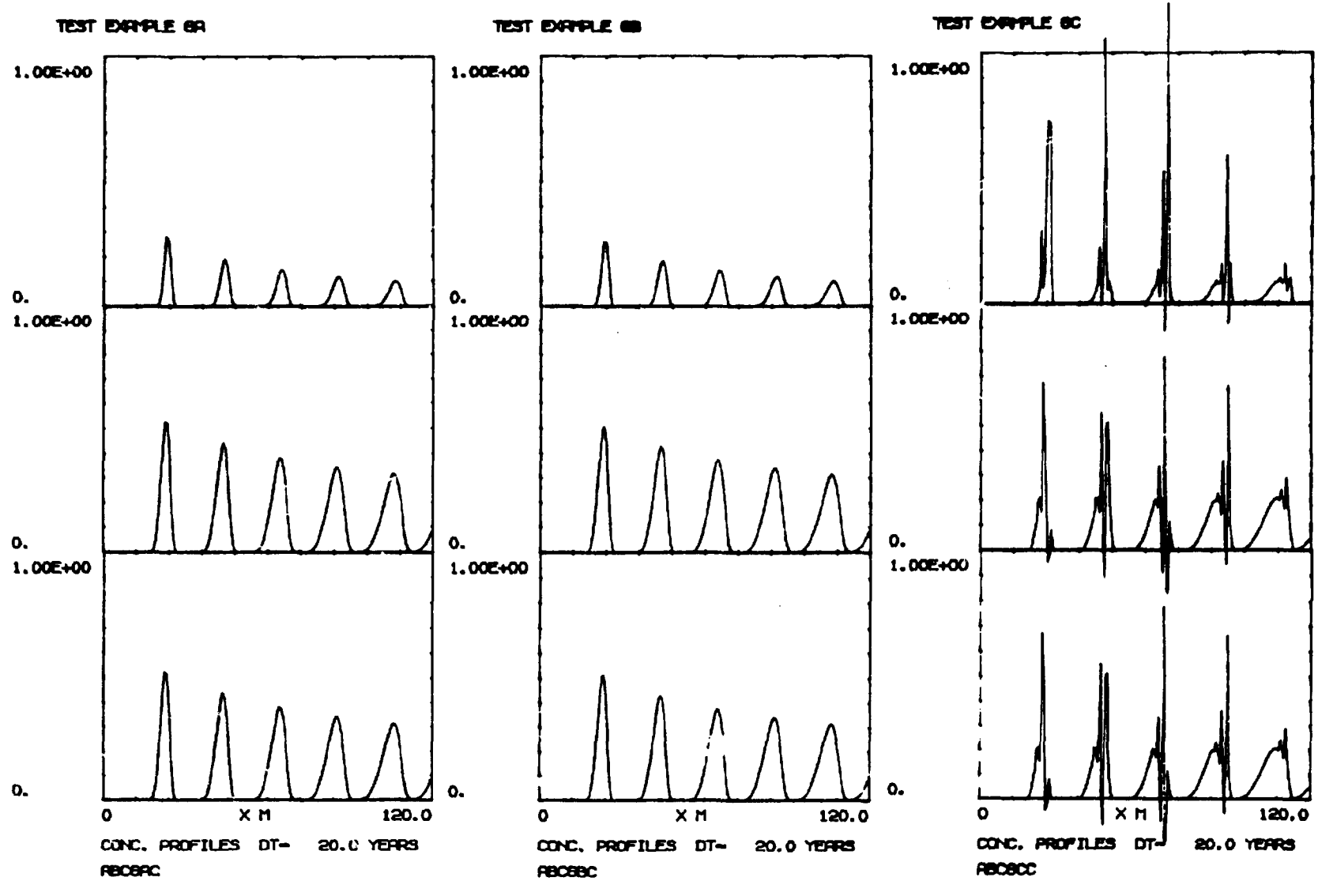

Fig. 6.10. Plotted output from test example 6A, 6B, and 6C

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